



Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 11:19 PM EDT

PDB ID : 5KCR / pdb_00005ker
EMDB ID : EMD-8237
Title : Cryo-EM structure of the Escherichia coli 70S ribosome in complex with antibiotic Avilamycin C, mRNA and P-site tRNA at 3.6Å resolution
Authors : Arenz, S.; Juette, M.F.; Graf, M.; Nguyen, F.; Huter, P.; Polikanov, Y.S.; Blanchard, S.C.; Wilson, D.N.
Deposited on : 2016-06-06
Resolution : 3.60 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

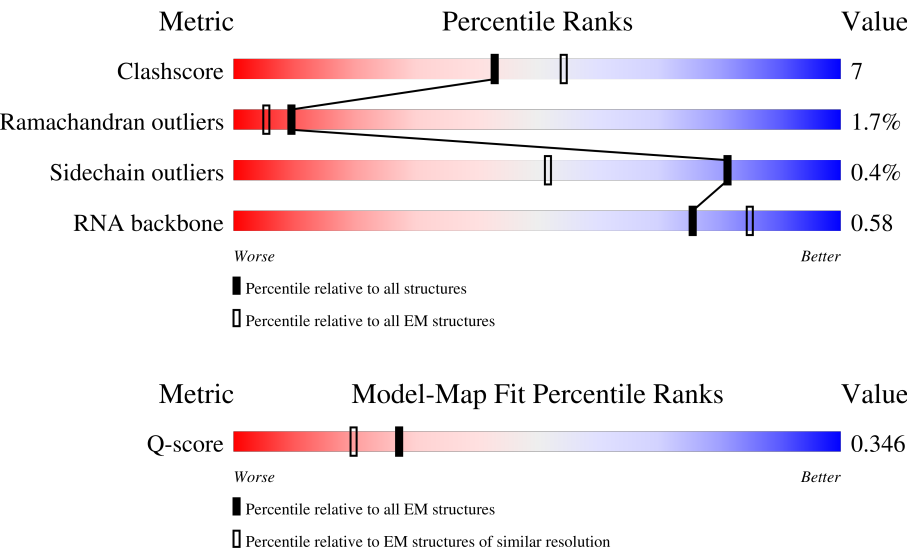
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12797 (3.10 - 4.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	2904	
2	1B	120	
3	1D	273	

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Mol	Chain	Length	Quality of chain
4	1E	209	
5	1F	201	
6	1G	179	
7	1H	177	
8	1I	149	
9	1J	165	
10	1K	142	
11	1N	142	
12	1O	123	
13	1P	144	
14	1Q	136	
15	1R	127	
16	1S	117	
17	1T	115	
18	1U	118	
19	1V	103	
20	1W	110	
21	1X	100	
22	1Y	104	
23	1Z	94	
24	10	85	
25	11	78	
26	12	63	
27	13	59	
28	15	57	

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Mol	Chain	Length	Quality of chain
29	16	55	
30	17	46	
31	18	65	
32	19	38	
33	1a	1539	
34	1b	241	
35	1c	233	
36	1d	206	
37	1e	167	
38	1f	135	
39	1g	179	
40	1h	130	
41	1i	130	
42	1j	103	
43	1k	129	
44	1l	124	
45	1m	118	
46	1n	101	
47	1o	89	
48	1p	82	
49	1q	84	
50	1r	75	
51	1s	92	
52	1t	87	
53	1u	71	

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Mol	Chain	Length	Quality of chain
54	1v	9	11%22%67%
55	1x	87	25%66%26%8%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 145689 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	2897	Total	C	N	O	P	8	0
			62361	27826	11476	20155	2904		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1A	1847	G	A	conflict	GB 802133627

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1D	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1E	209	Total	C	N	O	S	1	0
			1576	986	290	296	4		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1F	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1G	177	Total	C	N	O	S	0	0
			1404	896	246	256	6		

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1H	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1I	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1J	135	Total	C	N	O	S	0	0
			1023	648	179	192	4		

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1K	134	Total	C	N	O	S	0	0
			979	619	169	185	6		

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1N	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1O	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1P	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1Q	136	Total	C	N	O	S	2	0
			1090	696	211	177	6		

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1R	125	Total	C	N	O	S	0	0
			993	613	202	173	5		

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1S	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	1T	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	1U	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	1V	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1W	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1X	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1Y	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1Z	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	10	76	Total	C	N	O	S	1	0
			591	365	121	104	1		

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	11	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	12	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	13	58	Total	C	N	O	S	2	0
			463	290	90	81	2		

- Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	15	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 29 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	16	51	Total	C	N	O	S	0	0
			414	266	76	72			

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	17	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 31 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	18	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 32 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	19	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 33 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	1a	1539	Total	C	N	O	P	0	0
			33015	14725	6052	10699	1539		

- Molecule 34 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 35 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 36 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1d	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 37 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1e	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 38 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	1f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 39 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 40 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	1h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 41 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	1i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 42 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	1j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 43 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	1k	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 44 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 45 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 46 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	1n	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 47 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	1o	88	Total	C	N	O	S	0	0
			710	437	143	129	1		

- Molecule 48 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	1p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 49 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 50 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	1r	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 51 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	1s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 52 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	1t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 53 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	1u	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

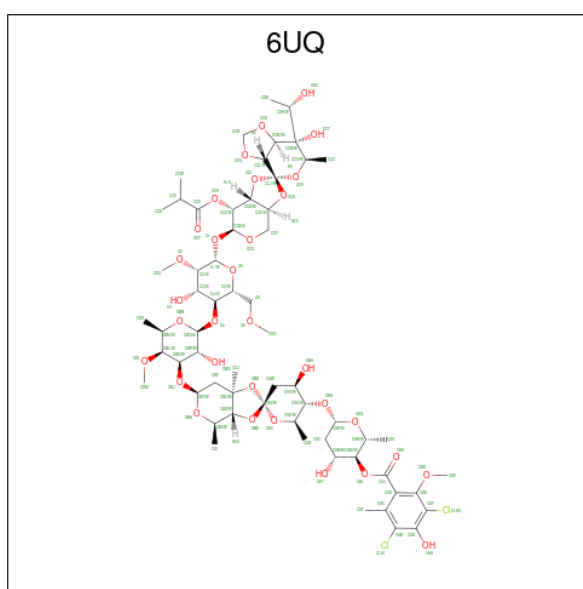
- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	1v	3	Total	C	N	O	P	0	0
			60	27	7	23	3		

- Molecule 55 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	1x	87	Total	C	N	O	P	0	0
			1861	829	333	612	87		

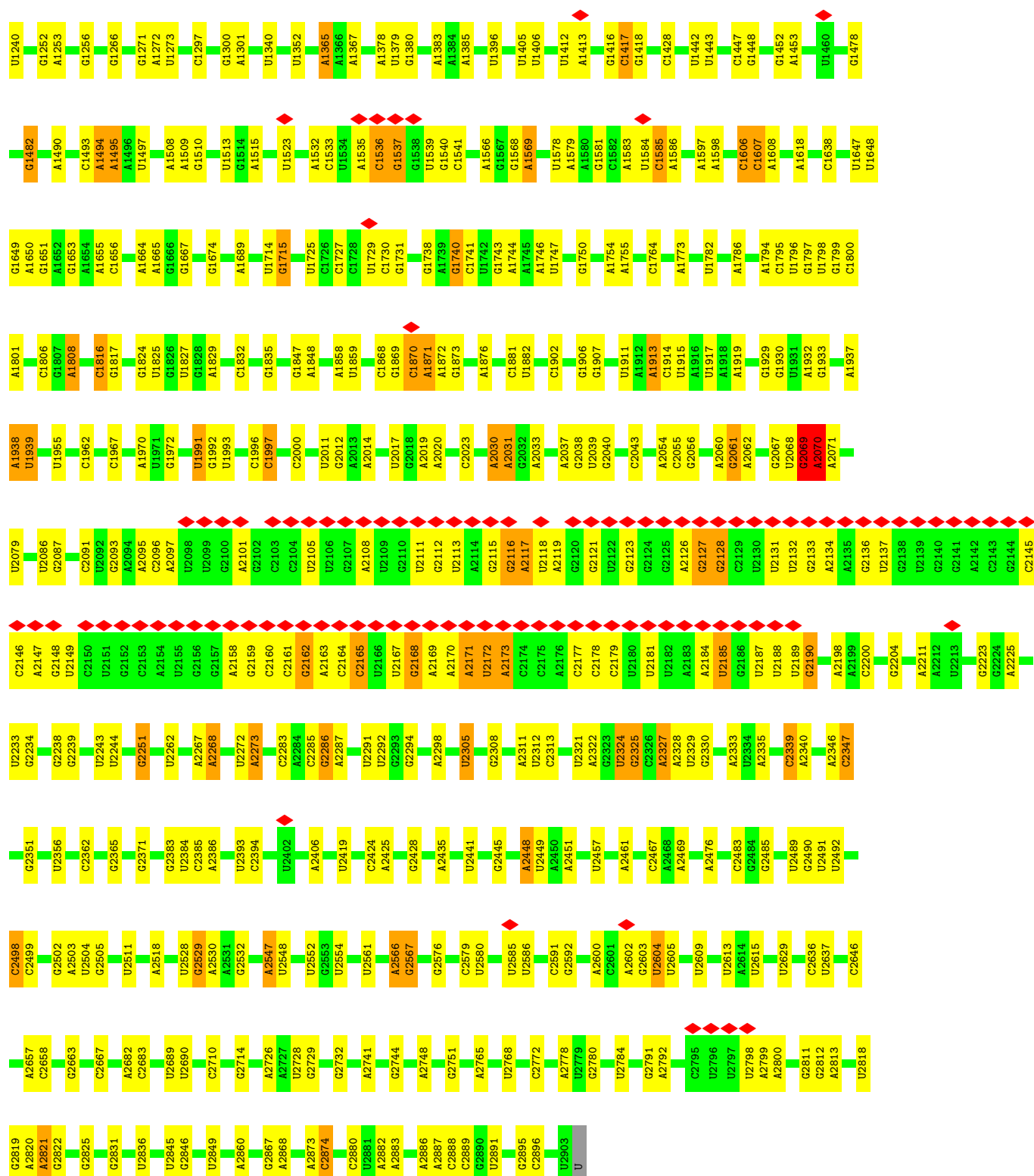
- Molecule 56 is (2R,3S,4R,6S)-4-hydroxy-6-{{[(2R,3aR,4R,4'R,5'S,6S,6'R,7aR)-4'-hydroxy-6-{{[(2S,3R,4R,5S,6R)-3-hydroxy-2-{{[(2R,3S,4S,5S,6S)-4-hydroxy-6-{{(2R,3aS,3a'R,6S,6'R,7R,7'R,7aR,7a'R)-7'-hydroxy-7'-[(1S)-1-hydroxyethyl]-6'-methyl-7-[(2-methylpropanoyl)oxy]octahydro-4H-2,4'-spirobi[[1,3]dioxolo[4,5-c]pyran]-6-yl}oxy)-5-methoxy-2-(methoxymethyl)tetrahydro-2H-pyran-3-yl}oxy}-5-methoxy-6-methyltetrahydro-2H-pyran-4-yl}oxy}-4,6',7a-trimethyloctahydro-4H-spiro[1,3-dioxolo[4,5-c]pyran-2,2'-pyran]-5'-yl}oxy}-2-methyltetrahydro-2H-pyran-3-yl 3,5-dichloro-4-hydroxy-2-methoxy-6-methylbenzoate (non-preferred name) (CCD ID: 6UQ) (formula: C₆₁H₉₀Cl₂O₃₂).



Mol	Chain	Residues	Atoms				AltConf
56	1A	1	Total	C	Cl	O	0
			95	61	2	32	

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

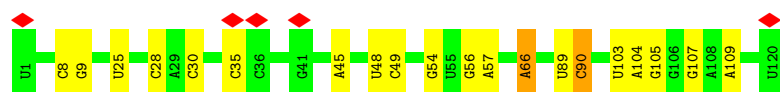
Mol	Chain	Residues	Atoms		AltConf
57	19	1	Total	Zn	0
			1	1	



• Molecule 2: 5S Ribosomal RNA

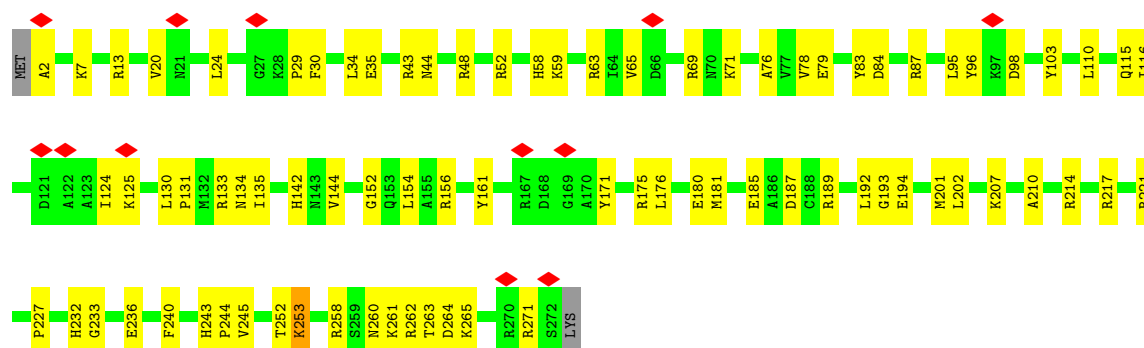
Chain 1B:





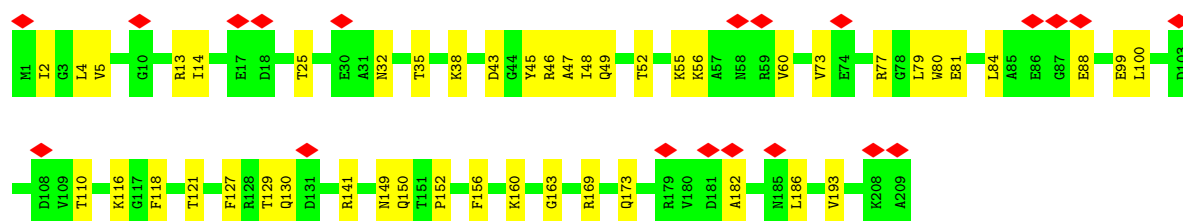
• Molecule 3: 50S ribosomal protein L2

Chain 1D: 70% 29%



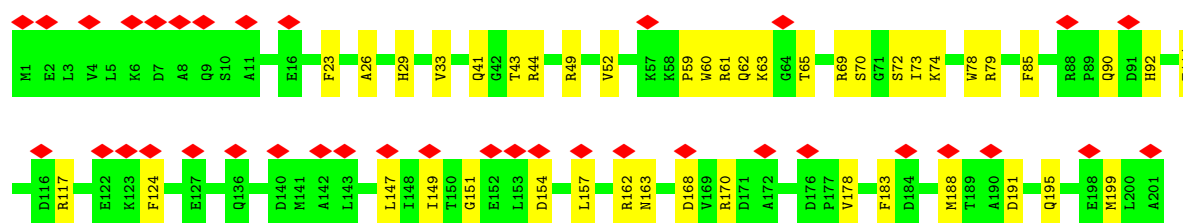
• Molecule 4: 50S ribosomal protein L3

Chain 1E: 10% 78% 22%



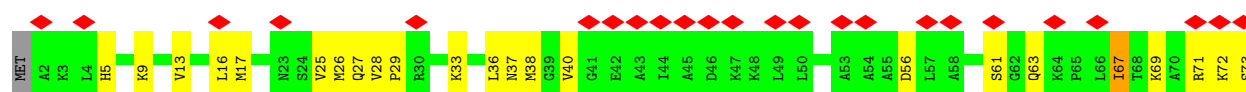
• Molecule 5: 50S ribosomal protein L4

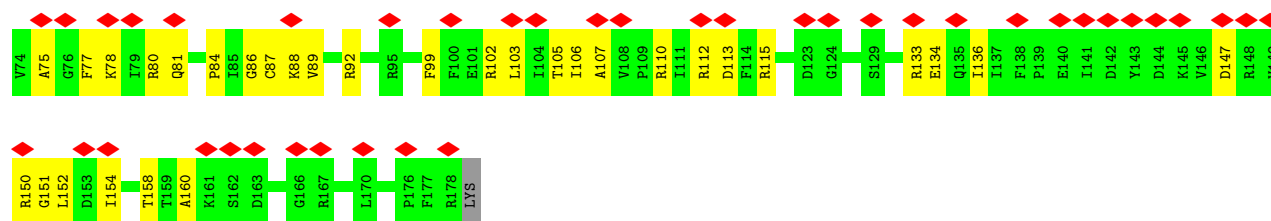
Chain 1F: 18% 79% 21%



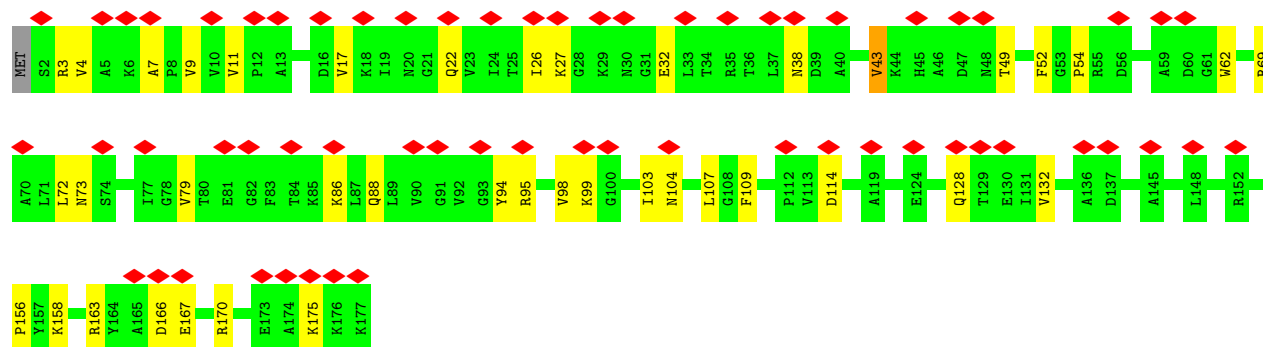
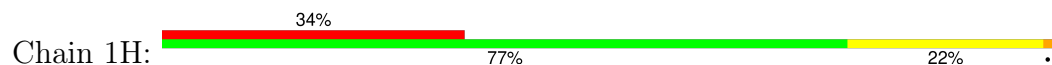
• Molecule 6: 50S ribosomal protein L5

Chain 1G: 36% 69% 30%

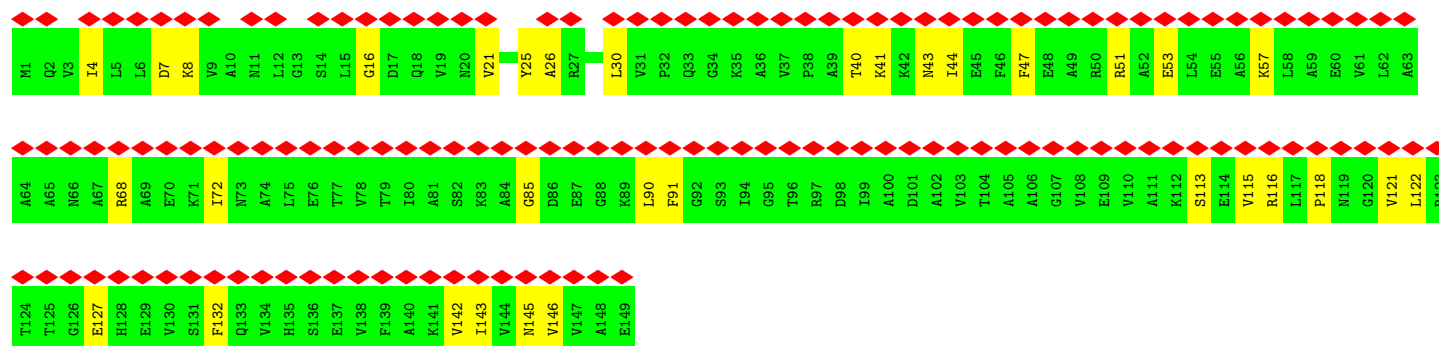
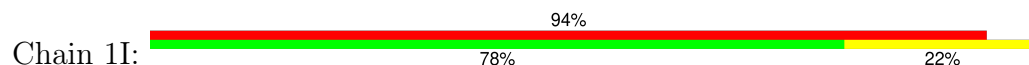




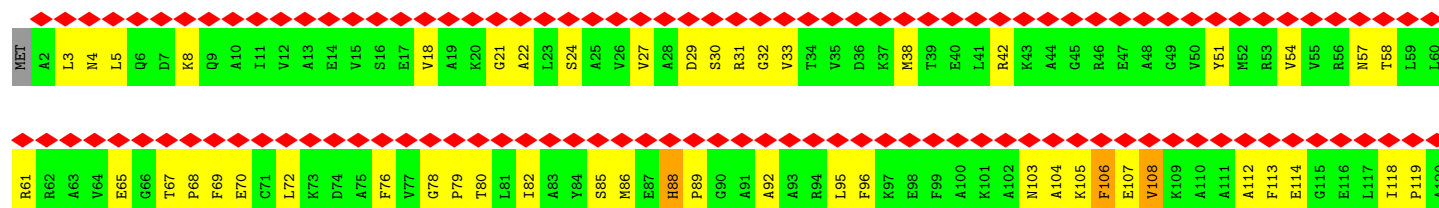
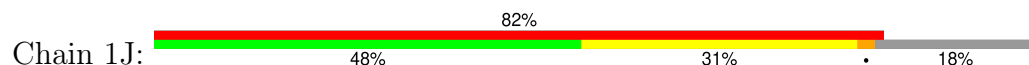
• Molecule 7: 50S ribosomal protein L6

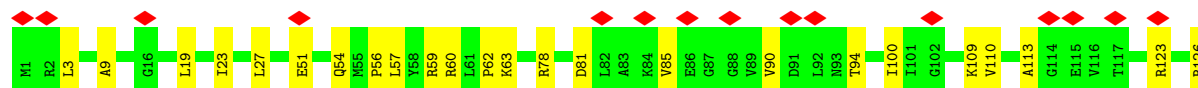


• Molecule 8: 50S ribosomal protein L9



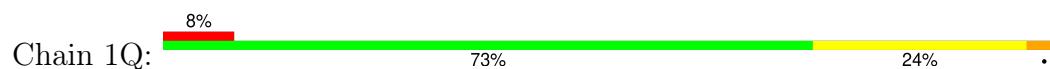
• Molecule 9: 50S ribosomal protein L10



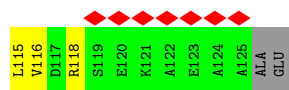




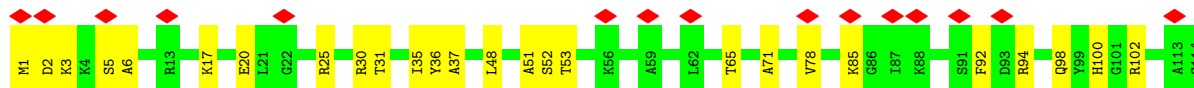
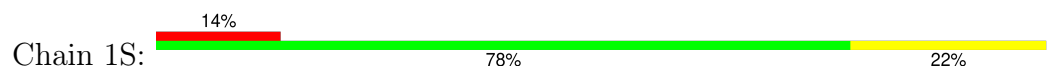
- Molecule 14: 50S ribosomal protein L16



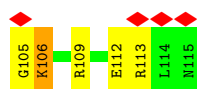
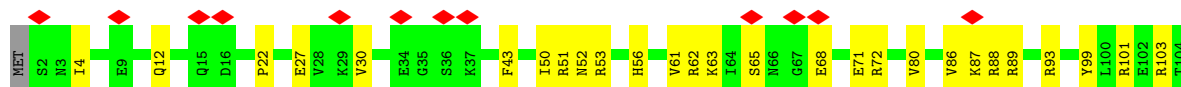
- Molecule 15: 50S ribosomal protein L17



- Molecule 16: 50S ribosomal protein L18

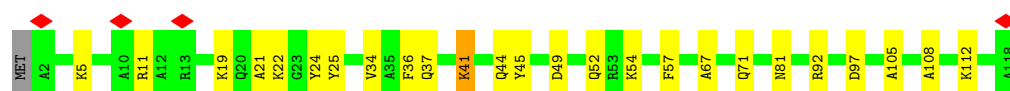


- Molecule 17: 50S ribosomal protein L19



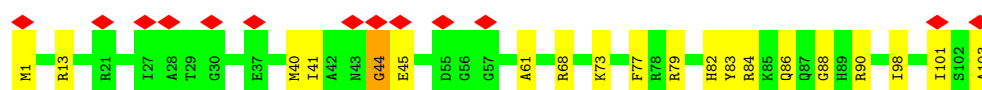
- Molecule 18: 50S ribosomal protein L20

Chain 1U:  78% 20% ..



- Molecule 19: 50S ribosomal protein L21

Chain 1V:  13% 81% 18% .



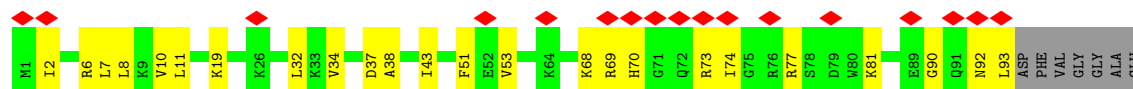
- Molecule 20: 50S ribosomal protein L22

Chain 1W:  10% 81% 19%



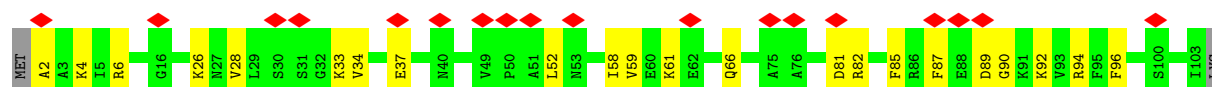
- Molecule 21: 50S ribosomal protein L23

Chain 1X:  17% 69% 24% 7%



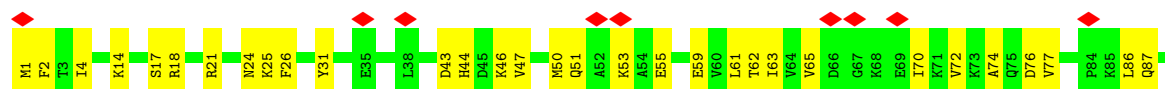
- Molecule 22: 50S ribosomal protein L24

Chain 1Y:  17% 77% 21% .



- Molecule 23: 50S ribosomal protein L25

Chain 1Z:  11% 66% 34%

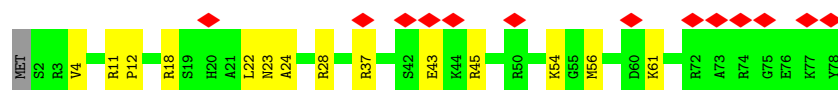
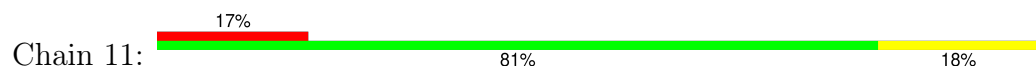


- Molecule 24: 50S ribosomal protein L27

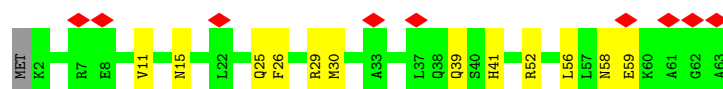
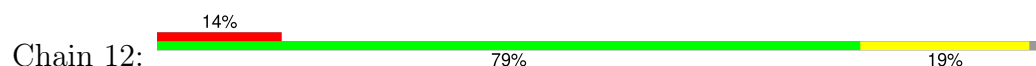
Chain 10:  6% 59% 29% 11%



- Molecule 25: 50S ribosomal protein L28



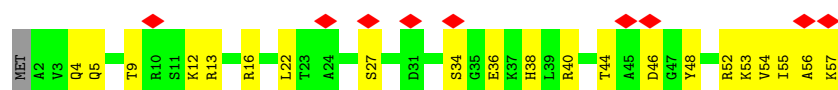
- Molecule 26: 50S ribosomal protein L29



- Molecule 27: 50S ribosomal protein L30



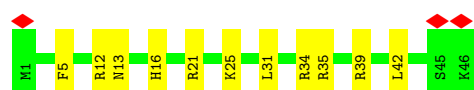
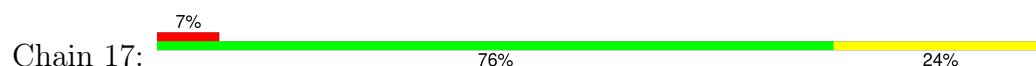
- Molecule 28: 50S ribosomal protein L32



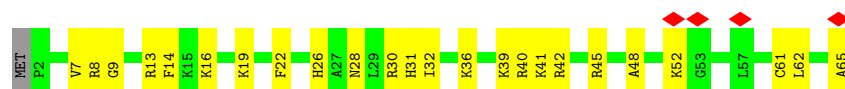
- Molecule 29: 50S ribosomal protein L33



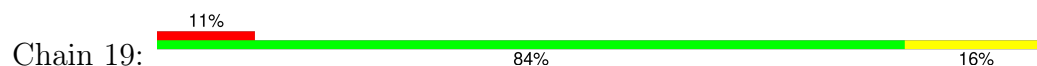
- Molecule 30: 50S ribosomal protein L34



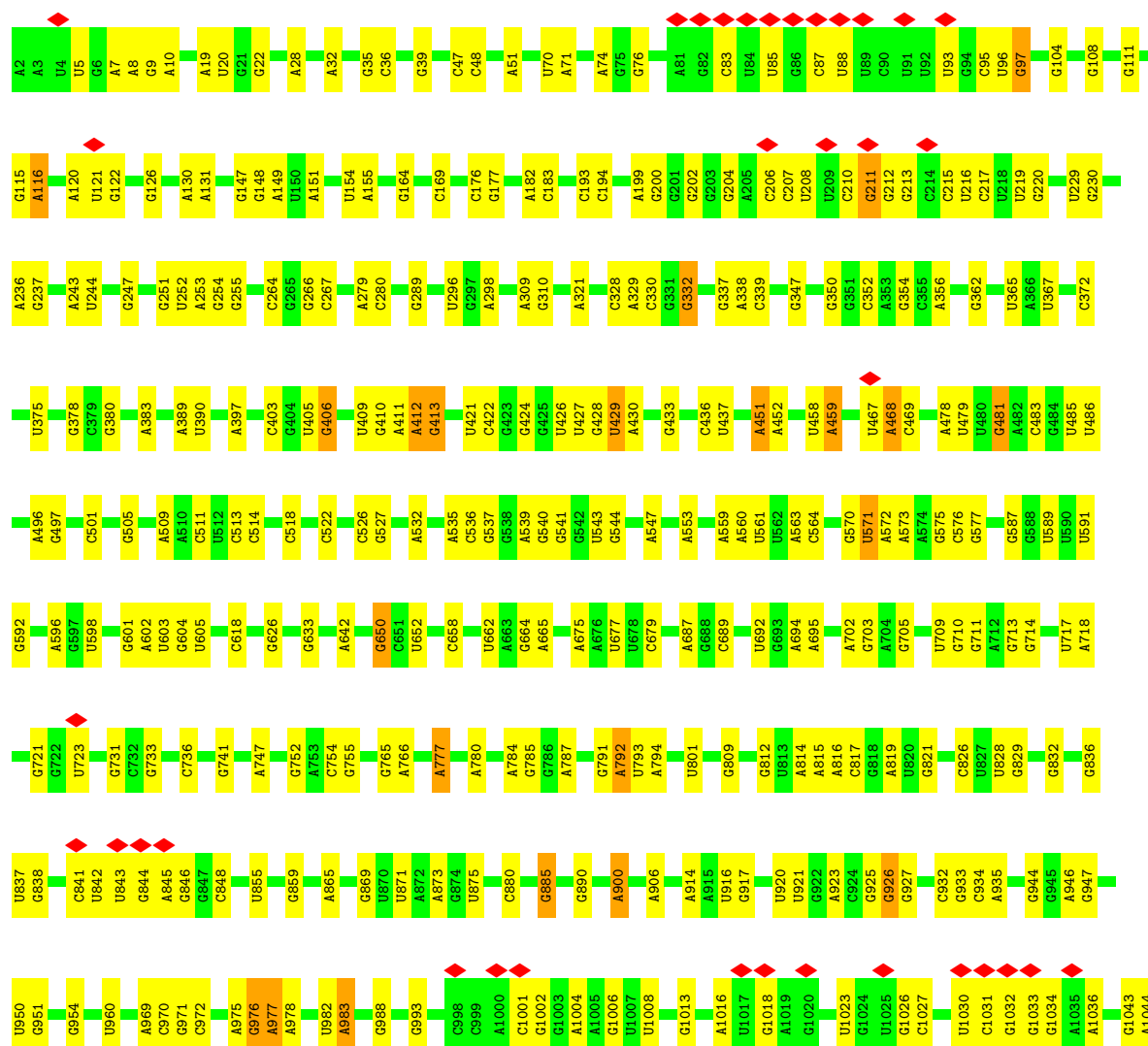
- Molecule 31: 50S ribosomal protein L35

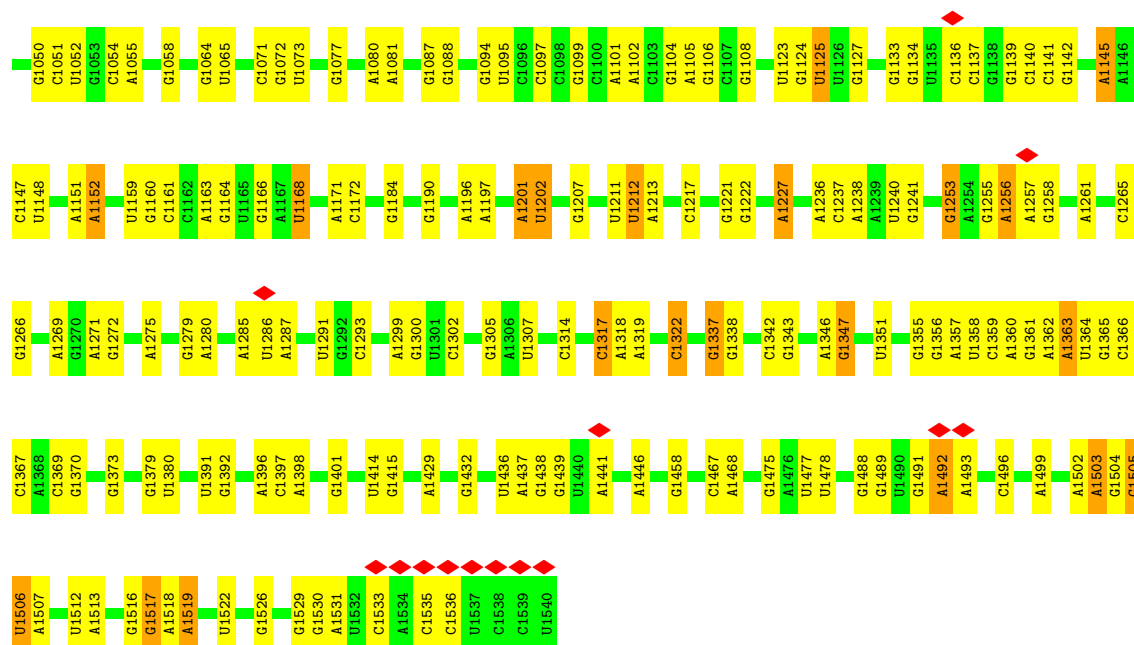


- Molecule 32: 50S ribosomal protein L36



- Molecule 33: 16S Ribosomal RNA





• Molecule 34: 30S ribosomal protein S2

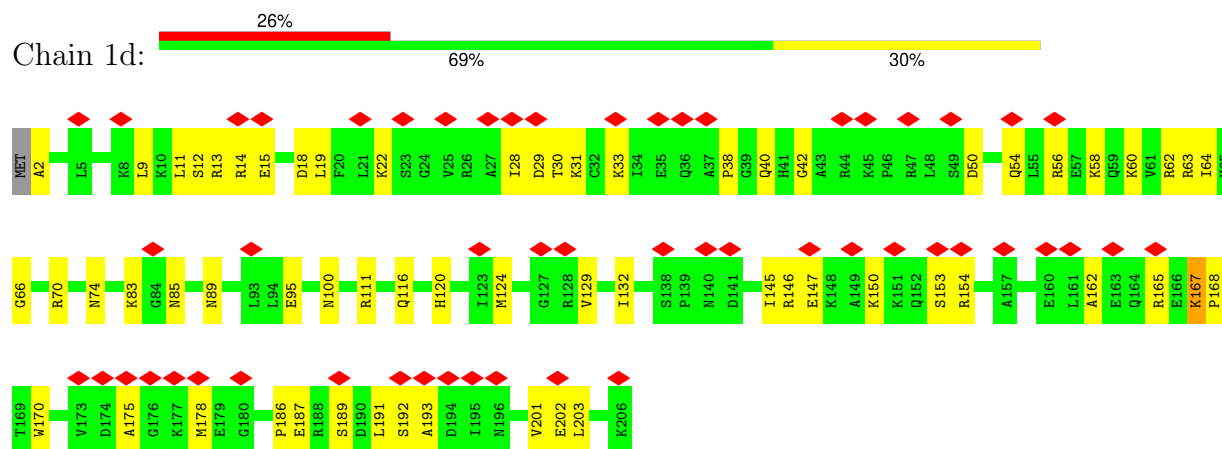


• Molecule 35: 30S ribosomal protein S3

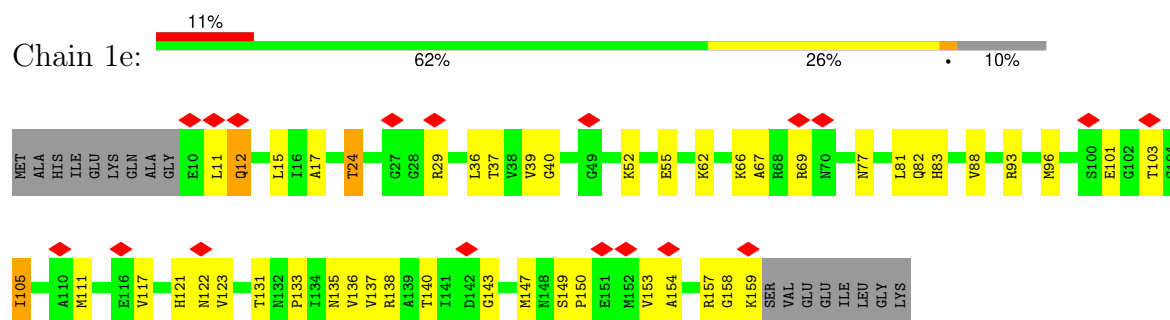




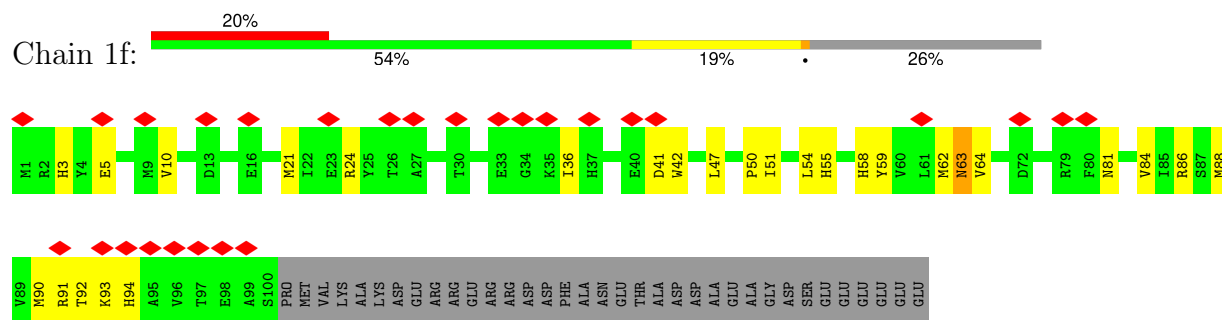
• Molecule 36: 30S ribosomal protein S4



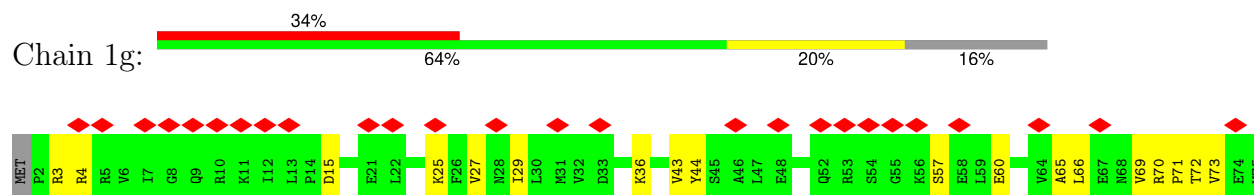
• Molecule 37: 30S ribosomal protein S5

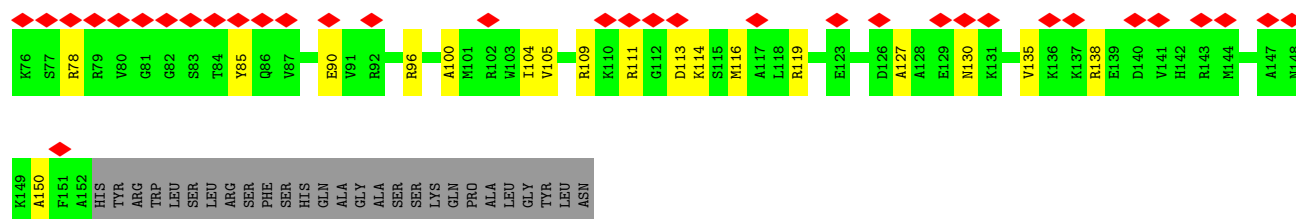


• Molecule 38: 30S ribosomal protein S6

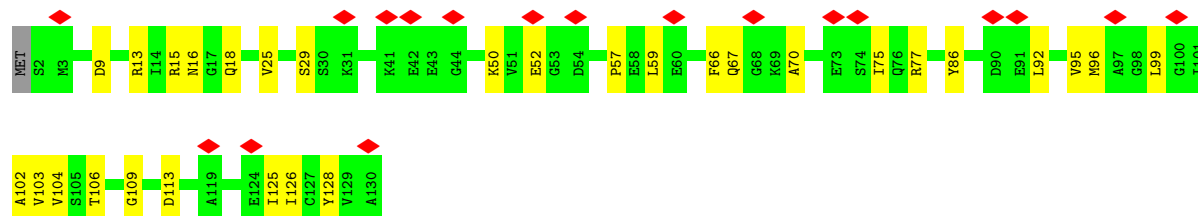
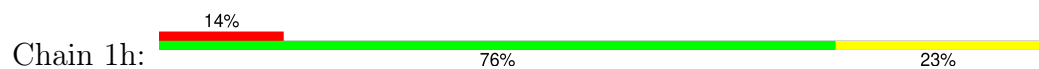


• Molecule 39: 30S ribosomal protein S7

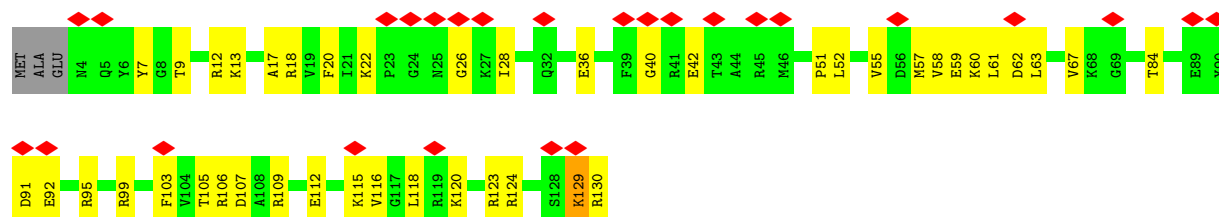




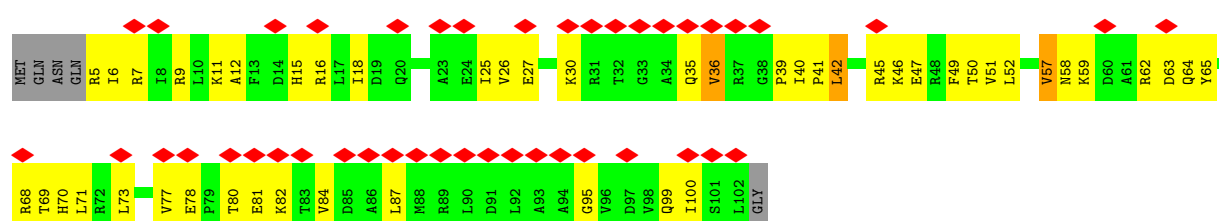
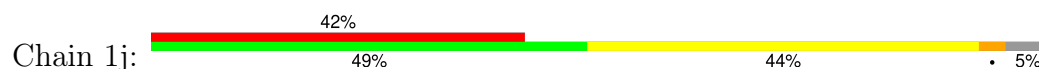
- Molecule 40: 30S ribosomal protein S8



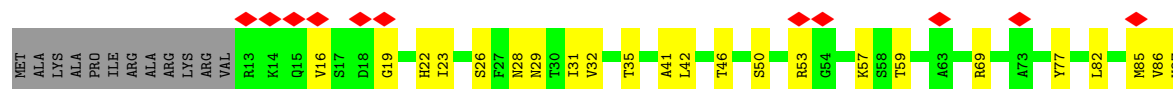
- Molecule 41: 30S ribosomal protein S9

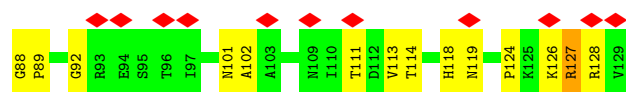


- Molecule 42: 30S ribosomal protein S10

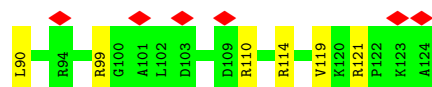


- Molecule 43: 30S ribosomal protein S11

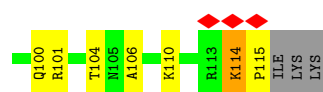
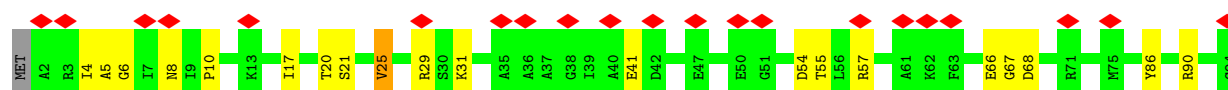
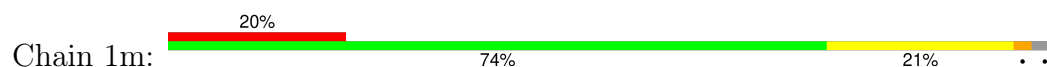




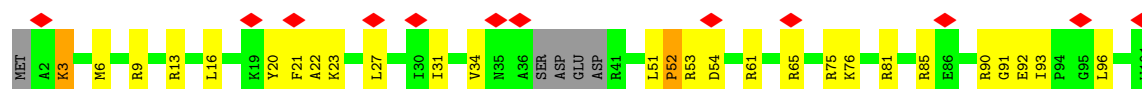
- Molecule 44: 30S ribosomal protein S12



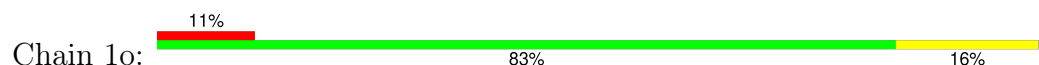
- Molecule 45: 30S ribosomal protein S13



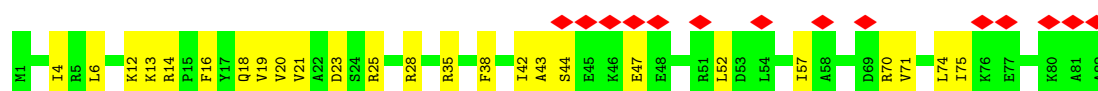
- Molecule 46: 30S ribosomal protein S14



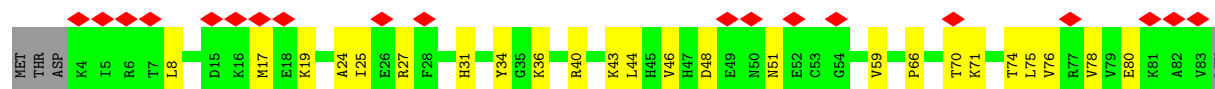
- Molecule 47: 30S ribosomal protein S15



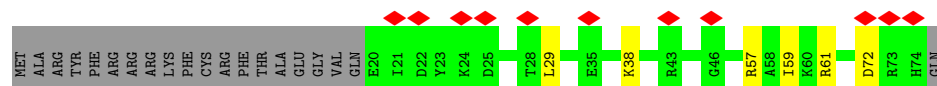
- Molecule 48: 30S ribosomal protein S16



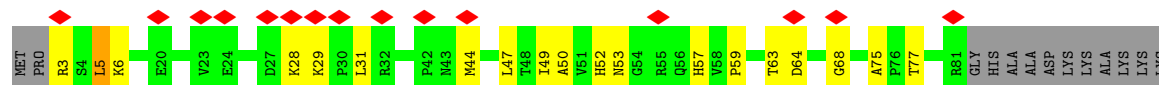
- Molecule 49: 30S ribosomal protein S17



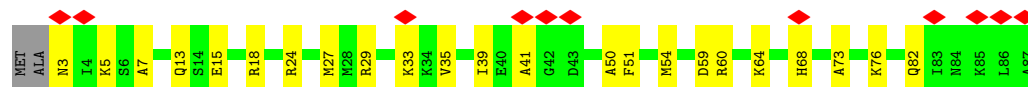
- Molecule 50: 30S ribosomal protein S18



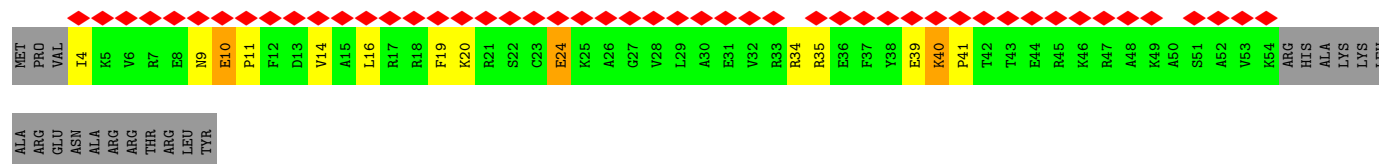
- Molecule 51: 30S ribosomal protein S19



- Molecule 52: 30S ribosomal protein S20



- Molecule 53: 30S ribosomal protein S21

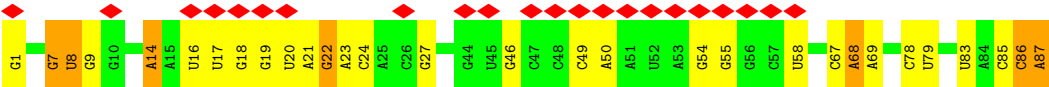


- Molecule 54: mRNA



- Molecule 55: P-site tRNA





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61651	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.004	Depositor
Minimum map value	-0.002	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.000801	Depositor
Map size (Å)	407.74402, 407.74402, 407.74402	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.108, 1.108, 1.108	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1MG, ZN, 2MA, H2U, MEQ, OMC, 6MZ, 5MC, 6UQ, G7M, 2MG, 5MU, OMU, PSU, OMG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1A	0.14	0/69297	0.34	1/108106 (0.0%)
2	1B	0.12	0/2872	0.29	0/4478
3	1D	0.19	0/2121	0.46	0/2852
4	1E	0.17	0/1576	0.39	0/2119
5	1F	0.17	0/1571	0.40	0/2113
6	1G	0.22	0/1428	0.44	0/1919
7	1H	0.18	0/1343	0.38	0/1816
8	1I	0.21	0/1121	0.43	0/1515
9	1J	0.26	0/1037	0.66	3/1400 (0.2%)
10	1K	0.23	0/993	0.52	0/1341
11	1N	0.36	0/1152	0.57	2/1551 (0.1%)
12	1O	0.20	0/955	0.43	0/1279
13	1P	0.19	0/1062	0.42	0/1413
14	1Q	0.20	0/1115	0.49	1/1488 (0.1%)
15	1R	0.18	0/1006	0.43	0/1345
16	1S	0.17	0/910	0.41	0/1219
17	1T	0.18	0/929	0.42	0/1242
18	1U	0.17	0/960	0.39	0/1278
19	1V	0.17	0/829	0.42	0/1107
20	1W	0.15	0/864	0.36	0/1156
21	1X	0.18	0/744	0.49	0/994
22	1Y	0.19	0/787	0.47	0/1051
23	1Z	0.19	0/766	0.40	0/1025
24	10	0.20	0/598	0.44	0/790
25	11	0.18	0/635	0.40	0/848
26	12	0.16	0/502	0.36	0/667
27	13	0.17	0/467	0.33	0/623
28	15	0.21	0/450	0.42	0/599
29	16	0.24	0/421	0.48	0/561
30	17	0.24	0/380	0.53	0/498
31	18	0.17	0/513	0.35	0/676
32	19	0.17	0/303	0.37	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	1a	0.11	0/36966	0.18	0/57666
34	1b	0.15	0/1735	0.36	0/2338
35	1c	0.13	0/1651	0.33	0/2225
36	1d	0.14	0/1665	0.37	0/2227
37	1e	0.15	0/1118	0.41	0/1504
38	1f	0.14	0/835	0.41	0/1128
39	1g	0.13	0/1195	0.33	0/1602
40	1h	0.17	0/989	0.34	0/1326
41	1i	0.16	0/1034	0.44	0/1375
42	1j	0.20	0/796	0.42	0/1077
43	1k	0.15	0/893	0.38	0/1205
44	1l	0.15	0/969	0.42	0/1300
45	1m	0.15	0/892	0.39	0/1193
46	1n	0.11	0/785	0.37	0/1043
47	1o	0.15	0/718	0.34	0/959
48	1p	0.15	0/659	0.37	0/884
49	1q	0.15	0/657	0.45	0/881
50	1r	0.14	0/462	0.34	0/621
51	1s	0.13	0/652	0.32	0/877
52	1t	0.13	0/671	0.35	0/888
53	1u	0.18	0/430	0.50	0/570
54	1v	0.18	0/65	0.32	0/98
55	1x	0.13	0/2080	0.26	0/3242
All	All	0.15	0/157624	0.33	7/235695 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	1N	0	1
27	13	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1Q	36	VAL	N-CA-C	-8.38	104.58	112.96
9	1J	132	TYR	N-CA-C	7.17	120.51	111.69
9	1J	132	TYR	CA-C-N	6.58	133.55	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	1J	132	TYR	C-N-CA	6.58	133.55	121.70
11	1N	136	GLN	CA-C-N	5.91	125.67	119.76
11	1N	136	GLN	C-N-CA	5.91	125.67	119.76
1	1A	2070	A	C1'-C2'-O2'	5.25	116.28	108.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	13	3[B]	LYS	Peptide
11	1N	135	GLN	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	62361	0	31379	423	0
2	1B	2569	0	1301	18	0
3	1D	2082	0	2154	67	0
4	1E	1576	0	1627	45	0
5	1F	1552	0	1619	40	0
6	1G	1404	0	1433	44	0
7	1H	1323	0	1371	32	0
8	1I	1110	0	1148	20	0
9	1J	1023	0	1050	53	0
10	1K	979	0	1028	36	0
11	1N	1129	0	1162	42	0
12	1O	946	0	1023	18	0
13	1P	1053	0	1129	24	0
14	1Q	1090	0	1183	32	0
15	1R	993	0	1034	28	0
16	1S	900	0	935	24	0
17	1T	917	0	962	38	0
18	1U	947	0	1019	25	0
19	1V	816	0	839	23	0
20	1W	857	0	922	15	0
21	1X	738	0	807	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	1Y	779	0	831	19	0
23	1Z	753	0	780	26	0
24	10	591	0	606	25	0
25	11	625	0	652	14	0
26	12	501	0	531	11	0
27	13	463	0	504	12	0
28	15	444	0	458	23	0
29	16	414	0	442	20	0
30	17	377	0	418	15	0
31	18	504	0	572	23	0
32	19	302	0	340	5	0
33	1a	33015	0	16617	252	0
34	1b	1704	0	1732	29	0
35	1c	1624	0	1696	35	0
36	1d	1643	0	1707	39	0
37	1e	1105	0	1148	30	0
38	1f	817	0	808	14	0
39	1g	1181	0	1238	25	0
40	1h	979	0	1031	21	0
41	1i	1022	0	1070	26	0
42	1j	786	0	828	37	0
43	1k	877	0	887	29	0
44	1l	955	0	1016	20	0
45	1m	883	0	941	18	0
46	1n	774	0	824	21	0
47	1o	710	0	728	12	0
48	1p	649	0	666	18	0
49	1q	648	0	691	16	0
50	1r	455	0	478	5	0
51	1s	637	0	665	11	0
52	1t	665	0	714	18	0
53	1u	425	0	449	11	0
54	1v	60	0	32	2	0
55	1x	1861	0	938	16	0
56	1A	95	0	0	2	0
57	19	1	0	0	0	0
All	All	145689	0	98163	1578	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (1578) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1J:22:ALA:HB2	9:1J:86:MET:SD	1.64	1.35
1:1A:1847:G:N2	1:1A:1848:A:H62	1.52	1.07
9:1J:22:ALA:CB	9:1J:86:MET:SD	2.48	1.02
1:1A:1847:G:H21	1:1A:1848:A:N6	1.63	0.97
1:1A:1799:G:OP1	3:1D:258:ARG:NH1	2.03	0.91
3:1D:65:VAL:HG21	3:1D:87:ARG:HH22	1.33	0.91
13:1P:62:PRO:HB2	31:18:30:ARG:HH11	1.36	0.88
33:1a:1127:G:H1	33:1a:1145:A:H61	1.21	0.88
1:1A:1083:U:H4'	9:1J:42:ARG:HH12	1.38	0.88
1:1A:827:U:H2'	1:1A:2068:U:C2	2.09	0.88
33:1a:1124:G:O2'	33:1a:1145:A:N6	2.06	0.87
18:1U:44:GLN:HE21	19:1V:77:PHE:HB3	1.40	0.86
1:1A:2116:G:O6	1:1A:2171:A:N6	2.08	0.85
6:1G:33:LYS:HD3	6:1G:92:ARG:HH11	1.41	0.85
1:1A:674:G:H1'	5:1F:69:ARG:HE	1.40	0.84
1:1A:2683:C:OP1	17:1T:51:ARG:NH2	2.11	0.84
1:1A:2285:C:OP2	29:16:6:ARG:NH2	2.12	0.83
10:1K:113:LYS:HB3	10:1K:117:MET:HE3	1.59	0.83
36:1d:100:ASN:OD1	36:1d:111:ARG:NH1	2.12	0.82
1:1A:1124:G:N3	32:19:37:GLN:NE2	2.28	0.82
8:1I:16:GLY:O	8:1I:51:ARG:NH2	2.12	0.81
9:1J:21:GLY:CA	9:1J:86:MET:HE1	2.10	0.81
9:1J:31:ARG:HH21	9:1J:79:PRO:HD3	1.43	0.80
1:1A:2419:U:OP1	31:18:41:LYS:NZ	2.13	0.80
5:1F:90:GLN:HE21	5:1F:92:HIS:HE1	1.30	0.80
11:1N:74:TYR:HD2	11:1N:92:MET:HG3	1.48	0.79
21:1X:38:ALA:O	21:1X:81:LYS:NZ	2.16	0.79
33:1a:765:G:H1	33:1a:812:G:HO2'	1.30	0.78
17:1T:63:LYS:NZ	17:1T:65:SER:OG	2.16	0.78
38:1f:90:MET:SD	50:1r:61:ARG:NH1	2.57	0.78
6:1G:158:THR:HG22	6:1G:160:ALA:H	1.48	0.78
16:1S:36:TYR:HD1	16:1S:52:SER:HB2	1.48	0.78
11:1N:31:GLU:HG2	11:1N:142:ILE:HG13	1.65	0.78
1:1A:320:A:N3	5:1F:163:ASN:ND2	2.31	0.78
30:17:34:ARG:HG3	30:17:39:ARG:HG3	1.66	0.77
1:1A:958:U:OP2	14:1Q:14:LYS:NZ	2.17	0.77
1:1A:2469:A:H1'	14:1Q:55:ARG:HH21	1.49	0.77
33:1a:1266:G:N2	33:1a:1269:A:OP2	2.16	0.77
1:1A:2822:G:O6	15:1R:2:ARG:NH1	2.17	0.77
1:1A:466:A:OP1	30:17:34:ARG:NH2	2.18	0.77
5:1F:117:ARG:NH2	5:1F:183:PHE:O	2.19	0.76
33:1a:362:G:N2	33:1a:365:U:OP2	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2845:U:O3'	17:1T:53:ARG:NH1	2.19	0.75
24:10:23:VAL:HB	24:10:26:PHE:HE1	1.51	0.75
1:1A:2384:U:OP2	24:10:55:ARG:NH2	2.19	0.75
33:1a:237:G:H4'	49:1q:27:ARG:HH12	1.51	0.75
42:1j:47:GLU:OE1	46:1n:76:LYS:NZ	2.20	0.75
9:1J:92:ALA:HB1	9:1J:96:PHE:HE2	1.52	0.75
23:1Z:21:ARG:NH2	23:1Z:87:GLN:O	2.20	0.75
29:16:21:TYR:OH	29:16:39:PHE:O	2.03	0.75
5:1F:147:LEU:HB2	5:1F:183:PHE:HD2	1.51	0.74
41:1i:112:GLU:OE2	41:1i:115:LYS:NZ	2.18	0.74
1:1A:1112:G:O3'	7:1H:3:ARG:NH1	2.20	0.74
1:1A:1266:G:OP2	28:15:16:ARG:NH1	2.15	0.74
33:1a:76:G:H1	33:1a:93:U:H3	1.36	0.74
42:1j:25:ILE:HD11	42:1j:87:LEU:HG	1.70	0.74
9:1J:21:GLY:C	9:1J:86:MET:HE1	2.13	0.74
33:1a:944:G:N1	33:1a:1338:G:OP2	2.21	0.74
1:1A:1847:G:H21	1:1A:1848:A:H62	0.77	0.73
37:1e:81:LEU:HD13	37:1e:123:VAL:HG11	1.68	0.73
28:15:46:ASP:O	28:15:53:LYS:NZ	2.21	0.73
45:1m:101:ARG:NH1	45:1m:104:THR:OG1	2.20	0.73
35:1c:19:ASN:ND2	46:1n:90:ARG:O	2.21	0.73
1:1A:1655:A:H1'	4:1E:118:PHE:CE2	2.24	0.73
33:1a:848:C:OP1	34:1b:37:LYS:NZ	2.22	0.73
16:1S:48:LEU:O	16:1S:85:LYS:NZ	2.21	0.72
29:16:25:LYS:NZ	29:16:32:GLU:O	2.22	0.72
3:1D:152:GLY:O	3:1D:156:ARG:NH2	2.20	0.72
1:1A:827:U:H2'	1:1A:2068:U:O2	1.90	0.72
21:1X:8:LEU:O	26:12:29:ARG:NH1	2.23	0.71
33:1a:10:A:OP2	37:1e:131:THR:OG1	2.07	0.71
22:1Y:28:VAL:HG12	22:1Y:34:VAL:HG12	1.71	0.71
29:16:6:ARG:HH21	29:16:26:ASN:HB2	1.54	0.71
1:1A:2561:U:O2'	12:1O:23:LYS:HG3	1.91	0.71
3:1D:124:ILE:HG23	3:1D:192:LEU:HD21	1.73	0.71
3:1D:171:TYR:HD1	3:1D:185:GLU:HA	1.56	0.71
1:1A:1508:A:O2'	1:1A:1509:A:O4'	2.08	0.71
7:1H:7:ALA:O	7:1H:69:ARG:NE	2.24	0.71
11:1N:31:GLU:HG2	11:1N:142:ILE:CG1	2.21	0.71
1:1A:568:U:H1'	1:1A:2030:6MZ:H9C1	1.72	0.71
8:1I:40:THR:OG1	8:1I:43:ASN:ND2	2.22	0.71
9:1J:22:ALA:N	9:1J:86:MET:HE1	2.06	0.71
26:12:11:VAL:O	26:12:15:ASN:ND2	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:728:G:H4'	3:1D:13:ARG:HD3	1.73	0.70
6:1G:112:ARG:NH1	6:1G:134:GLU:OE2	2.23	0.70
33:1a:380:G:N2	33:1a:383:A:OP2	2.21	0.70
1:1A:920:A:OP1	27:13:19:LYS:NZ	2.24	0.70
14:1Q:67:VAL:HG12	14:1Q:100:LYS:HD3	1.73	0.70
33:1a:1125:U:H4'	42:1j:7:ARG:HH12	1.54	0.70
34:1b:68:LEU:HD12	34:1b:154:MET:HE1	1.73	0.70
1:1A:1816:C:N4	3:1D:35:GLU:OE1	2.21	0.70
1:1A:1655:A:H1'	4:1E:118:PHE:HE2	1.56	0.70
1:1A:2371:G:O2'	29:16:46:HIS:ND1	2.24	0.70
44:1l:34:CYS:HA	44:1l:55:VAL:HA	1.73	0.70
28:15:13:ARG:HG3	28:15:16:ARG:HH12	1.57	0.70
33:1a:970:C:OP1	42:1j:59:LYS:NZ	2.25	0.70
35:1c:14:ILE:HG22	35:1c:15:VAL:HG13	1.74	0.70
1:1A:2305:U:C2	6:1G:151:GLY:HA3	2.27	0.70
39:1g:78:ARG:HB2	39:1g:85:TYR:HB2	1.73	0.70
55:1x:8:U:H3	55:1x:14:A:H62	1.40	0.70
1:1A:2223:G:O3'	3:1D:265:LYS:NZ	2.25	0.70
41:1i:92:GLU:OE1	41:1i:95:ARG:NH1	2.25	0.70
33:1a:618:C:O2'	48:1p:14:ARG:NH2	2.24	0.70
2:1B:57:A:H4'	6:1G:27:GLN:HE21	1.57	0.69
20:1W:4:ILE:HG12	20:1W:106:VAL:HG22	1.73	0.69
9:1J:22:ALA:CA	9:1J:86:MET:SD	2.80	0.69
13:1P:62:PRO:HB2	31:18:30:ARG:NH1	2.07	0.69
1:1A:2069:G7M:O2'	1:1A:2070:A:O5'	2.11	0.69
11:1N:23:LYS:NZ	11:1N:142:ILE:OXT	2.24	0.69
1:1A:301:G:OP2	22:1Y:82:ARG:NH1	2.25	0.69
11:1N:118:MET:HA	11:1N:121:LYS:NZ	2.06	0.69
38:1f:91:ARG:HH21	38:1f:93:LYS:HD3	1.57	0.69
23:1Z:26:PHE:HE2	23:1Z:44:HIS:HA	1.58	0.69
3:1D:78:VAL:HG21	3:1D:110:LEU:HD21	1.72	0.69
1:1A:136:G:H1	1:1A:143:C:N4	1.91	0.68
1:1A:2846:G:P	17:1T:53:ARG:HH12	2.16	0.68
35:1c:129:MET:SD	35:1c:132:ARG:NH1	2.66	0.68
1:1A:2602:A:O2'	55:1x:85:C:O5'	2.11	0.68
33:1a:1077:G:N2	33:1a:1080:A:OP2	2.27	0.68
1:1A:1252:G:H1	18:1U:37:GLN:HE21	1.41	0.68
1:1A:1798:U:OP2	3:1D:271:ARG:NH2	2.25	0.68
1:1A:2658:C:OP1	7:1H:158:LYS:NZ	2.27	0.68
1:1A:706:A:OP1	3:1D:7:LYS:NZ	2.26	0.68
16:1S:71:ALA:HB2	16:1S:102:ARG:HG3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1H:52:PHE:CE2	7:1H:69:ARG:HA	2.28	0.68
16:1S:36:TYR:CD1	16:1S:52:SER:HB2	2.29	0.68
1:1A:714:U:O4	47:1o:89:ARG:NH2	2.27	0.68
10:1K:100:LYS:HB2	10:1K:141:GLU:HB2	1.76	0.68
12:1O:38:ILE:HD11	12:1O:112:PHE:HZ	1.58	0.68
34:1b:130:THR:HG22	34:1b:132:LYS:H	1.59	0.68
1:1A:287:G:H1	1:1A:353:C:H42	1.42	0.68
11:1N:74:TYR:CD2	11:1N:92:MET:HG3	2.29	0.68
1:1A:1340:U:OP1	21:1X:19:LYS:NZ	2.27	0.67
24:10:43:THR:HG23	24:10:57:HIS:HD2	1.58	0.67
44:1l:5:ASN:HD21	49:1q:36:LYS:HE2	1.59	0.67
9:1J:22:ALA:N	9:1J:86:MET:CE	2.57	0.67
29:16:38:LYS:HB2	29:16:49:TYR:HE2	1.59	0.67
37:1e:77:ASN:HB2	37:1e:82:GLN:HG2	1.76	0.67
35:1c:11:ARG:NH1	35:1c:180:ALA:O	2.27	0.67
50:1r:72:ASP:OD2	53:1u:4:ILE:N	2.28	0.67
7:1H:99:LYS:NZ	7:1H:104:ASN:OD1	2.19	0.67
42:1j:80:THR:HG22	42:1j:82:LYS:H	1.59	0.67
44:1l:68:GLY:O	44:1l:99:ARG:NH1	2.25	0.67
11:1N:13:ARG:NH1	11:1N:49:ASP:O	2.27	0.67
1:1A:2467:C:OP2	32:19:4:ARG:NH2	2.27	0.67
33:1a:1351:U:O4	41:1i:120:LYS:NZ	2.26	0.67
1:1A:2483:C:N3	14:1Q:123:LYS:NZ	2.37	0.67
7:1H:95:ARG:HD2	7:1H:128:GLN:HB3	1.76	0.67
33:1a:570:G:O6	33:1a:865:A:N6	2.28	0.67
33:1a:1359:C:OP2	46:1n:75:ARG:NH1	2.27	0.67
1:1A:2741:A:O3'	32:19:36:ARG:NH1	2.28	0.67
34:1b:219:ALA:O	34:1b:222:ARG:NH1	2.28	0.67
36:1d:38:PRO:HD2	36:1d:42:GLY:HA3	1.77	0.67
33:1a:809:G:OP2	47:1o:48:LYS:NZ	2.28	0.66
14:1Q:50:ARG:O	14:1Q:52:ALA:N	2.28	0.66
1:1A:1153:C:OP1	18:1U:92:ARG:NH2	2.28	0.66
3:1D:115:GLN:O	3:1D:125:LYS:NZ	2.27	0.66
33:1a:717:U:H4'	43:1k:119:ASN:HD22	1.61	0.66
21:1X:53:VAL:HG12	21:1X:92:ASN:HD22	1.61	0.66
1:1A:846:U:O2'	1:1A:847:U:OP2	2.13	0.66
7:1H:52:PHE:HE2	7:1H:69:ARG:HA	1.59	0.66
35:1c:34:ASP:OD2	46:1n:65:ARG:NH1	2.27	0.66
41:1i:123:ARG:NH1	41:1i:124:ARG:O	2.29	0.66
29:16:38:LYS:HB2	29:16:49:TYR:CE2	2.31	0.66
33:1a:406:G:H21	36:1d:116:GLN:HE22	1.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1a:501:C:OP1	44:1l:114:ARG:NH2	2.28	0.66
1:1A:1095:A:H61	10:1K:30:GLN:HE22	1.44	0.66
1:1A:1653:G:H3'	15:1R:2:ARG:HD2	1.78	0.66
15:1R:55:ALA:HA	15:1R:80:PHE:CE1	2.31	0.66
12:1O:98:ARG:NH1	33:1a:339:C:OP2	2.29	0.66
14:1Q:47:GLU:OE1	14:1Q:50:ARG:NH1	2.30	0.65
9:1J:31:ARG:HE	9:1J:79:PRO:HG3	1.61	0.65
23:1Z:51:GLN:HE22	23:1Z:86:LEU:HD21	1.61	0.65
42:1j:5:ARG:HG3	42:1j:6:ILE:HG13	1.77	0.65
18:1U:97:ASP:OD2	19:1V:13:ARG:NE	2.30	0.65
45:1m:4:ILE:HD11	45:1m:10:PRO:HD2	1.77	0.65
30:17:31:LEU:HB3	30:17:35:ARG:HH12	1.61	0.65
39:1g:113:ASP:HB2	39:1g:119:ARG:HG2	1.78	0.65
34:1b:10:LEU:HD12	34:1b:43:LEU:HD22	1.78	0.65
24:10:21:LEU:HD11	24:10:41[A]:ARG:HE	1.61	0.65
1:1A:2294:G:H5'	16:1S:98:GLN:HE22	1.61	0.65
5:1F:62:GLN:HE22	5:1F:69:ARG:HD2	1.62	0.65
9:1J:21:GLY:C	9:1J:86:MET:CE	2.69	0.65
34:1b:163:VAL:HG21	34:1b:173:ILE:HD11	1.79	0.65
36:1d:95:GLU:HG2	36:1d:186:PRO:HG3	1.76	0.65
38:1f:81:ASN:HB3	38:1f:84:VAL:HG12	1.79	0.65
33:1a:1317:C:N3	46:1n:53:ARG:NH1	2.45	0.65
39:1g:71:PRO:O	39:1g:96:ARG:NH1	2.30	0.65
10:1K:56:PRO:HD3	10:1K:75:PRO:HD3	1.78	0.64
20:1W:73:LYS:HB2	20:1W:106:VAL:HB	1.78	0.64
1:1A:1824:G:H5''	3:1D:52:ARG:HH11	1.62	0.64
33:1a:1124:G:HO2'	33:1a:1145:A:H62	1.42	0.64
17:1T:52:ASN:O	17:1T:53:ARG:NH1	2.31	0.64
25:11:18:ARG:HH21	25:11:24:ALA:HB2	1.61	0.64
36:1d:54:GLN:NE2	36:1d:202:GLU:OE1	2.28	0.64
11:1N:37:ARG:HD3	11:1N:39:LYS:HD3	1.80	0.64
11:1N:49:ASP:OD2	11:1N:121:LYS:NZ	2.30	0.64
23:1Z:63:ILE:HD11	23:1Z:91:PHE:CD2	2.33	0.64
1:1A:2127:G:O2'	1:1A:2128:G:O4'	2.15	0.64
33:1a:859:G:OP2	33:1a:869:G:N1	2.27	0.64
2:1B:48:U:P	16:1S:30:ARG:HH22	2.20	0.64
9:1J:132:TYR:H	9:1J:133:GLU:HB2	1.63	0.64
13:1P:81:ASP:HB3	13:1P:100:ILE:HD13	1.80	0.64
33:1a:104:G:OP2	52:1t:13:GLN:NE2	2.29	0.64
52:1t:5:LYS:HG3	52:1t:7:ALA:H	1.63	0.64
1:1A:7:G:O4'	11:1N:135:GLN:NE2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1795:C:O2	3:1D:253:LYS:NZ	2.30	0.64
1:1A:2127:G:O2'	1:1A:2128:G:O5'	2.15	0.64
13:1P:23:ILE:HG12	19:1V:82:HIS:CD2	2.32	0.64
15:1R:32:GLU:HG2	15:1R:115:LEU:HD12	1.79	0.64
1:1A:2768:U:O2'	11:1N:95:ARG:NH2	2.31	0.63
33:1a:1127:G:H1	33:1a:1145:A:N6	1.94	0.63
39:1g:57:SER:HB3	39:1g:60:GLU:HG2	1.80	0.63
9:1J:132:TYR:N	9:1J:133:GLU:HB2	2.12	0.63
1:1A:6:A:O2'	11:1N:135:GLN:NE2	2.29	0.63
1:1A:1151:A:H4'	18:1U:81:ASN:ND2	2.13	0.63
5:1F:90:GLN:HE21	5:1F:92:HIS:CE1	2.14	0.63
33:1a:436:C:O2'	36:1d:154:ARG:NH1	2.31	0.63
33:1a:1097:C:OP1	34:1b:139:ARG:NH2	2.31	0.63
1:1A:444:C:OP2	5:1F:44:ARG:NH2	2.32	0.63
33:1a:875:U:O2'	40:1h:15:ARG:NH1	2.31	0.63
1:1A:45:G:H5''	1:1A:46:G:H5'	1.80	0.63
1:1A:1568:G:O4'	3:1D:58:HIS:HE1	1.80	0.63
5:1F:59:PRO:HG2	5:1F:78:TRP:HH2	1.64	0.63
33:1a:1006:G:N2	33:1a:1023:U:O2	2.31	0.63
38:1f:21:MET:HG2	38:1f:24:ARG:HH21	1.61	0.63
2:1B:9:G:P	16:1S:25:ARG:HH12	2.22	0.63
17:1T:51:ARG:CZ	17:1T:53:ARG:HG3	2.29	0.63
22:1Y:85:PHE:HE1	22:1Y:94:ARG:HG2	1.63	0.63
23:1Z:26:PHE:CE2	23:1Z:44:HIS:HA	2.33	0.63
33:1a:664:G:H22	33:1a:741:G:H1	1.46	0.63
1:1A:2365:G:N7	31:18:39:LYS:NZ	2.41	0.62
8:1I:68:ARG:O	8:1I:72:ILE:HG12	2.00	0.62
21:1X:2:ILE:HG22	21:1X:7:LEU:HD21	1.80	0.62
8:1I:115:VAL:HG13	8:1I:132:PHE:HE1	1.63	0.62
33:1a:1071:C:H42	33:1a:1104:G:H1	1.47	0.62
36:1d:95:GLU:HA	36:1d:100:ASN:HD22	1.65	0.62
1:1A:1252:G:H1	18:1U:37:GLN:NE2	1.96	0.62
9:1J:24:SER:OG	9:1J:85:SER:OG	2.09	0.62
15:1R:30:ARG:NH2	15:1R:72:ASP:OD2	2.32	0.62
1:1A:2511:U:H1'	4:1E:130:GLN:HE21	1.64	0.62
6:1G:110:ARG:NH1	6:1G:136:ILE:O	2.32	0.62
3:1D:76:ALA:HB2	3:1D:96:TYR:CD1	2.35	0.62
9:1J:21:GLY:HA3	9:1J:86:MET:HE1	1.81	0.62
9:1J:69:PHE:HB3	9:1J:72:LEU:HD12	1.82	0.62
28:15:54:VAL:HG23	28:15:55:ILE:HG12	1.80	0.62
23:1Z:17:SER:HB3	23:1Z:21:ARG:HH12	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:1m:86:TYR:OH	45:1m:90:ARG:NH2	2.33	0.62
33:1a:1081:A:OP2	37:1e:52:LYS:NZ	2.33	0.62
14:1Q:17:ASN:O	14:1Q:38:ARG:NH1	2.32	0.61
40:1h:92:LEU:HD21	40:1h:113:ASP:HB2	1.80	0.61
48:1p:20:VAL:HG12	48:1p:35:ARG:HA	1.81	0.61
1:1A:65:U:H4'	21:1X:73:ARG:HE	1.65	0.61
15:1R:73:ASN:HA	15:1R:76:VAL:HG22	1.82	0.61
28:15:27:SER:HB2	28:15:40:ARG:HD3	1.83	0.61
40:1h:18:GLN:HE21	40:1h:70:ALA:HB1	1.65	0.61
29:16:13:SER:HA	29:16:49:TYR:CD1	2.35	0.61
33:1a:1439:G:OP2	52:1t:33:LYS:NZ	2.33	0.61
33:1a:405:U:O4	36:1d:2:ALA:N	2.34	0.61
42:1j:45:ARG:HB3	42:1j:69:THR:HB	1.81	0.61
17:1T:30:VAL:HG11	17:1T:72:ARG:HH22	1.65	0.60
42:1j:46:LYS:HG2	42:1j:68:ARG:HG2	1.82	0.60
12:1O:43:ILE:HD12	12:1O:56:ASP:HB2	1.83	0.60
1:1A:550:C:H2'	1:1A:551:G:H5''	1.83	0.60
7:1H:54:PRO:HG3	7:1H:62:TRP:CE2	2.37	0.60
19:1V:44:GLY:O	19:1V:45:GLU:HG2	2.01	0.60
9:1J:4:ASN:OD1	9:1J:5:LEU:N	2.33	0.60
39:1g:135:VAL:HA	39:1g:138:ARG:HG2	1.84	0.60
1:1A:715:A:H1'	47:1o:60:VAL:CG1	2.32	0.60
56:1A:3001:6UQ:OAK	56:1A:3001:6UQ:OAT	2.20	0.60
6:1G:63:GLN:HE21	6:1G:89:VAL:HG13	1.67	0.60
23:1Z:2:PHE:HB2	23:1Z:61:LEU:HD22	1.82	0.60
37:1e:133:PRO:HA	37:1e:136:VAL:HG12	1.84	0.60
44:1l:57:LEU:HD12	44:1l:61:PHE:HB2	1.82	0.60
49:1q:31:HIS:HD2	49:1q:34:TYR:H	1.47	0.60
6:1G:99:PHE:HA	6:1G:102:ARG:HE	1.66	0.60
17:1T:106:LYS:HE3	17:1T:109:ARG:HH22	1.66	0.60
44:1l:54:ARG:HA	44:1l:64:THR:HA	1.84	0.60
33:1a:1359:C:O2'	33:1a:1361:G:N7	2.34	0.60
9:1J:18:VAL:HG11	9:1J:51:TYR:CD2	2.37	0.59
9:1J:22:ALA:N	9:1J:86:MET:SD	2.75	0.59
11:1N:37:ARG:NH1	11:1N:44:TYR:OH	2.35	0.59
33:1a:1502:A:H62	33:1a:1505:G:H1	1.49	0.59
43:1k:126:LYS:O	53:1u:34:ARG:NE	2.35	0.59
15:1R:79:LEU:HD23	15:1R:83:LEU:HD12	1.84	0.59
1:1A:2200:C:OP2	25:11:37:ARG:NH1	2.36	0.59
21:1X:92:ASN:O	21:1X:93:LEU:HB2	2.01	0.59
39:1g:69:VAL:HG23	39:1g:100:ALA:HB1	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:878:A:N6	1:1A:899:A:O2'	2.35	0.59
33:1a:1058:G:OP1	35:1c:199:LYS:NZ	2.34	0.59
33:1a:537:G:H5''	44:1l:110:ARG:HH12	1.67	0.59
43:1k:88:GLY:H	43:1k:114:THR:HG22	1.67	0.59
17:1T:88:ARG:NH2	17:1T:112:GLU:HB2	2.17	0.59
40:1h:29:SER:HB2	40:1h:59:LEU:HB2	1.82	0.59
1:1A:545:U:H2'	1:1A:546:U:O3'	2.02	0.59
1:1A:1919:A:O2'	33:1a:1517:G:N3	2.28	0.59
6:1G:73:SER:OG	6:1G:81:GLN:N	2.36	0.59
10:1K:12:GLN:HG2	10:1K:56:PRO:HB3	1.85	0.59
45:1m:31:LYS:NZ	45:1m:41:GLU:OE1	2.35	0.59
7:1H:104:ASN:ND2	7:1H:114:ASP:OD1	2.36	0.59
10:1K:103:ARG:HA	10:1K:106:LEU:HD12	1.84	0.59
10:1K:113:LYS:O	10:1K:117:MET:N	2.36	0.59
5:1F:41:GLN:HG2	5:1F:43:THR:HG23	1.85	0.58
30:17:16:HIS:HA	30:17:21:ARG:HH22	1.68	0.58
33:1a:791:G:O6	33:1a:792:A:N6	2.36	0.58
41:1i:84:THR:HG21	41:1i:103:PHE:HB3	1.85	0.58
9:1J:119:PRO:HG2	9:1J:122:GLN:HB2	1.85	0.58
31:18:31:HIS:ND1	31:18:32:ILE:HG13	2.19	0.58
33:1a:1491:G:OP1	44:1l:44:LYS:NZ	2.30	0.58
43:1k:28:ASN:O	43:1k:57:LYS:NZ	2.36	0.58
5:1F:73:ILE:HA	5:1F:78:TRP:CZ3	2.38	0.58
9:1J:3:LEU:O	9:1J:8:LYS:NZ	2.37	0.58
11:1N:56:VAL:HB	11:1N:124:VAL:HG12	1.85	0.58
22:1Y:59:VAL:HG11	22:1Y:61:LYS:HE3	1.85	0.58
39:1g:73:VAL:HG12	39:1g:90:GLU:HA	1.85	0.58
1:1A:6:A:C2'	11:1N:135:GLN:HE22	2.16	0.58
2:1B:103:U:HO2'	23:1Z:31:TYR:HH	1.49	0.58
1:1A:84:A:OP1	22:1Y:6:ARG:NH1	2.36	0.58
1:1A:1606:C:H5'	1:1A:1607:C:OP1	2.03	0.58
1:1A:2886[A]:A:N1	28:15:40:ARG:HD2	2.18	0.58
5:1F:52:VAL:HB	5:1F:74:LYS:HD2	1.85	0.58
1:1A:858:G:OP1	24:10:78:LYS:NZ	2.23	0.58
12:1O:107:LEU:O	12:1O:109:SER:N	2.37	0.58
33:1a:8:A:N6	36:1d:202:GLU:O	2.34	0.58
1:1A:95:A:O2'	26:12:41:HIS:ND1	2.32	0.58
15:1R:63:ARG:HA	15:1R:80:PHE:CE2	2.39	0.58
15:1R:96:ARG:HH12	15:1R:116:VAL:HG13	1.68	0.58
1:1A:2070:A:H2'	1:1A:2071:A:C8	2.39	0.58
3:1D:227:PRO:HA	3:1D:233:GLY:HA2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1a:1001:C:H2'	33:1a:1002:G:H8	1.69	0.58
34:1b:12:ALA:HB1	34:1b:15:HIS:HE1	1.68	0.58
30:17:34:ARG:CD	30:17:42:LEU:HA	2.34	0.58
1:1A:1482:G:H1'	1:1A:1509:A:H61	1.68	0.57
33:1a:243:A:H4'	33:1a:244:U:H3'	1.86	0.57
33:1a:390:U:O3'	48:1p:28:ARG:NH1	2.37	0.57
1:1A:536:G:H4'	18:1U:57:PHE:CZ	2.39	0.57
42:1j:57:VAL:HG22	42:1j:58:ASN:H	1.68	0.57
2:1B:90:C:H5'	14:1Q:18[A]:ARG:HG2	1.87	0.57
3:1D:175:ARG:HE	3:1D:181:MET:HE1	1.69	0.57
17:1T:51:ARG:NH1	17:1T:56:HIS:O	2.37	0.57
33:1a:976:G:N2	33:1a:1362:A:O2'	2.38	0.57
9:1J:61:ARG:NH2	9:1J:76:PHE:O	2.37	0.57
1:1A:250:G:O5'	13:1P:59:ARG:NH1	2.37	0.57
1:1A:1113:U:H5'	7:1H:3:ARG:HH12	1.69	0.57
3:1D:84:ASP:OD2	3:1D:87:ARG:NH2	2.20	0.57
7:1H:88:GLN:HE21	7:1H:163:ARG:HD2	1.69	0.57
8:1I:41:LYS:HA	8:1I:44:ILE:HG22	1.86	0.57
1:1A:2780:G:P	11:1N:120:ARG:HE	2.27	0.57
9:1J:92:ALA:HB1	9:1J:96:PHE:CE2	2.36	0.57
14:1Q:54:THR:O	14:1Q:59:ARG:HG3	2.04	0.57
36:1d:11:LEU:HB3	36:1d:63:ARG:HD3	1.86	0.57
30:17:31:LEU:HB3	30:17:35:ARG:NH1	2.18	0.57
3:1D:260:ASN:OD1	3:1D:262:ARG:HG2	2.04	0.57
15:1R:87:PHE:HB3	15:1R:94:TYR:CE1	2.40	0.57
24:10:23:VAL:HB	24:10:26:PHE:CE1	2.37	0.57
1:1A:1664:A:H2	12:1O:1:MET:HE1	1.70	0.57
1:1A:2324:U:H3'	1:1A:2325:G:C5'	2.35	0.57
2:1B:103:U:O2'	23:1Z:31:TYR:OH	2.22	0.57
5:1F:59:PRO:HG2	5:1F:78:TRP:CH2	2.39	0.57
20:1W:23:LEU:HD21	28:15:22:LEU:HB2	1.86	0.57
10:1K:21:SER:HB3	10:1K:22:PRO:HD3	1.87	0.56
1:1A:282:A:H2'	1:1A:283:G:C8	2.40	0.56
2:1B:30:C:OP1	16:1S:3:LYS:NZ	2.30	0.56
5:1F:147:LEU:HB2	5:1F:183:PHE:CD2	2.37	0.56
43:1k:22:HIS:NE2	43:1k:85:MET:SD	2.79	0.56
1:1A:930:G:H1'	27:13:25:LEU:HD21	1.87	0.56
1:1A:1825:U:H4'	3:1D:232:HIS:HE1	1.70	0.56
10:1K:110:ALA:O	10:1K:114:ALA:N	2.39	0.56
33:1a:255:G:H4'	49:1q:19:LYS:HE3	1.88	0.56
55:1x:68:A:H5''	55:1x:69:A:OP2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:141:G:OP2	1:1A:142:A:N6	2.38	0.56
1:1A:1365:A:P	25:11:28:ARG:HH22	2.28	0.56
48:1p:18:GLN:HA	48:1p:38:PHE:HA	1.86	0.56
1:1A:747:5MU:H4'	20:1W:92:ARG:HH21	1.71	0.56
1:1A:2849:U:P	17:1T:93:ARG:HH21	2.29	0.56
6:1G:33:LYS:HB3	6:1G:92:ARG:HE	1.71	0.56
22:1Y:87:PHE:HE1	22:1Y:92:LYS:HE2	1.70	0.56
28:15:38:HIS:HB3	28:15:44:THR:HG22	1.86	0.56
33:1a:1307:U:OP1	45:1m:100:GLN:NE2	2.38	0.56
41:1i:92:GLU:HB3	41:1i:95:ARG:HH12	1.70	0.56
1:1A:784:G:H5'	1:1A:785:G:OP1	2.06	0.56
21:1X:69:ARG:HG2	21:1X:74:ILE:HG22	1.87	0.56
37:1e:150:PRO:HB3	40:1h:99:LEU:HD21	1.86	0.56
38:1f:3:HIS:H	38:1f:92:THR:HG23	1.70	0.56
43:1k:23:ILE:HD11	43:1k:86:VAL:HG22	1.87	0.56
52:1t:29:ARG:O	52:1t:33:LYS:HG2	2.06	0.56
1:1A:1536:C:H4'	1:1A:1537:G:H5''	1.88	0.56
1:1A:2011:U:OP1	20:1W:42:LYS:NZ	2.25	0.56
24:10:43:THR:HG23	24:10:57:HIS:CD2	2.39	0.56
41:1i:36:GLU:HA	41:1i:40:GLY:HA3	1.88	0.56
1:1A:1046:A:O2'	9:1J:8:LYS:HE3	2.05	0.56
2:1B:8:C:O3'	16:1S:25:ARG:NH1	2.38	0.56
8:1I:7:ASP:OD1	8:1I:8:LYS:N	2.39	0.56
46:1n:21:PHE:O	46:1n:23:LYS:N	2.39	0.56
52:1t:35:VAL:HG22	52:1t:50:ALA:HB1	1.88	0.56
12:1O:80:ASP:N	17:1T:68:GLU:OE2	2.39	0.56
26:12:52:ARG:O	26:12:56:LEU:HG	2.06	0.56
42:1j:63:ASP:OD2	46:1n:85:ARG:NH1	2.39	0.56
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.71	0.55
5:1F:178:VAL:HG23	13:1P:3:LEU:HD21	1.88	0.55
11:1N:117:ALA:HA	11:1N:120:ARG:HH21	1.71	0.55
22:1Y:81:ASP:OD1	22:1Y:82:ARG:N	2.35	0.55
23:1Z:43:ASP:OD2	23:1Z:46:LYS:HG2	2.05	0.55
36:1d:147:GLU:HA	36:1d:150:LYS:HE2	1.88	0.55
51:1s:31:LEU:H	51:1s:49:ILE:HA	1.71	0.55
1:1A:1176:U:H2'	1:1A:1177:G:C8	2.42	0.55
4:1E:121:THR:HB	4:1E:127:PHE:CD2	2.41	0.55
33:1a:28:A:O2'	33:1a:296:U:OP1	2.22	0.55
46:1n:27:LEU:HA	46:1n:31:ILE:HD13	1.88	0.55
1:1A:871:U:H2'	1:1A:872:U:C6	2.42	0.55
1:1A:2813:A:H2	1:1A:2887[B]:A:H61	1.51	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1T:99:TYR:O	17:1T:103:ARG:NH1	2.39	0.55
36:1d:29:ASP:O	36:1d:31:LYS:N	2.40	0.55
53:1u:10:GLU:HG3	53:1u:11:PRO:HD3	1.88	0.55
1:1A:790:U:O4	5:1F:61:ARG:NH2	2.39	0.55
1:1A:2886[B]:A:H2'	1:1A:2886[B]:A:N3	2.21	0.55
12:1O:58:LEU:HA	12:1O:89:ASN:OD1	2.06	0.55
16:1S:2:ASP:OD1	16:1S:5:SER:OG	2.18	0.55
16:1S:30:ARG:HG3	16:1S:102:ARG:HD2	1.88	0.55
17:1T:62:ARG:NH2	17:1T:71:GLU:OE2	2.39	0.55
17:1T:89:ARG:HB3	17:1T:113:ARG:NH1	2.22	0.55
35:1c:111:LEU:HB3	35:1c:204:LYS:HE3	1.88	0.55
55:1x:1:G:H1	55:1x:83:U:H3	1.55	0.55
1:1A:2393:U:H5''	13:1P:62:PRO:HB3	1.88	0.55
7:1H:86:LYS:HG2	7:1H:132:VAL:HG22	1.87	0.55
33:1a:926:G:N2	54:1v:16:C:OP1	2.32	0.55
1:1A:1170:C:H2'	1:1A:1171:G:C8	2.41	0.55
2:1B:54:G:H21	6:1G:26:MET:HE3	1.72	0.55
4:1E:48:ILE:HG23	4:1E:84:LEU:HD21	1.88	0.55
29:16:21:TYR:HE2	29:16:38:LYS:HB2	1.72	0.55
1:1A:1689:A:H4'	33:1a:1475:G:H4'	1.89	0.55
20:1W:25:ARG:NH2	20:1W:74:ILE:O	2.30	0.55
33:1a:254:G:H4'	49:1q:71:LYS:HZ1	1.71	0.55
33:1a:954:G:H21	33:1a:1227:A:N6	2.04	0.55
33:1a:1001:C:H2'	33:1a:1002:G:C8	2.42	0.55
1:1A:2298:A:OP1	6:1G:71:ARG:NH2	2.37	0.55
1:1A:2313:C:H5''	6:1G:88:LYS:HD2	1.89	0.55
3:1D:154:LEU:HD13	3:1D:176:LEU:HD21	1.88	0.55
7:1H:27:LYS:NZ	7:1H:32:GLU:OE1	2.39	0.55
10:1K:113:LYS:O	10:1K:117:MET:HG2	2.07	0.55
21:1X:11:LEU:HD23	21:1X:34:VAL:HG12	1.88	0.55
34:1b:166:ALA:HB3	34:1b:191:SER:HB3	1.88	0.55
1:1A:729:G:OP2	3:1D:207:LYS:NZ	2.27	0.55
4:1E:127:PHE:HZ	4:1E:160:LYS:HB2	1.72	0.55
6:1G:67:ILE:HG22	6:1G:87:CYS:HB3	1.89	0.55
9:1J:118:ILE:HG22	9:1J:123:ILE:HG12	1.88	0.55
22:1Y:26:LYS:HD2	22:1Y:37:GLU:HG2	1.88	0.55
33:1a:526:C:OP2	44:1l:88:LYS:NZ	2.35	0.55
33:1a:1105:A:H2'	33:1a:1106:G:H8	1.72	0.55
1:1A:922:C:H1'	24:10:26:PHE:CD2	2.42	0.54
1:1A:2172:U:H4'	1:1A:2173:A:H5'	1.88	0.54
1:1A:2330:G:O3'	24:10:44:LYS:NZ	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2849:U:OP1	17:1T:93:ARG:NH2	2.36	0.54
4:1E:116:LYS:HA	15:1R:1:MET:SD	2.47	0.54
20:1W:109:ASP:OD1	20:1W:110:ARG:N	2.40	0.54
34:1b:145:GLU:OE1	34:1b:152:LYS:NZ	2.37	0.54
1:1A:2251:OMG:OP1	14:1Q:81[A]:ARG:NH2	2.40	0.54
35:1c:150:LYS:HG3	35:1c:169:ARG:HB3	1.88	0.54
40:1h:50:LYS:HG2	40:1h:52:GLU:HG2	1.89	0.54
44:1l:114:ARG:HG3	44:1l:119:VAL:HB	1.88	0.54
47:1o:26:GLU:OE2	47:1o:77:ARG:NH2	2.40	0.54
13:1P:51:GLU:OE1	13:1P:60:ARG:NH2	2.39	0.54
33:1a:988:G:N2	33:1a:1217:C:O2	2.41	0.54
1:1A:2602:A:N3	55:1x:85:C:OP2	2.40	0.54
1:1A:2636:C:O2'	4:1E:45:TYR:OH	2.23	0.54
33:1a:437:U:O2'	36:1d:120:HIS:ND1	2.40	0.54
1:1A:1754:A:O2'	17:1T:103:ARG:NH2	2.39	0.54
4:1E:186:LEU:HD21	17:1T:4:ILE:HG21	1.90	0.54
33:1a:1396:A:O2'	37:1e:29:ARG:NH2	2.40	0.54
41:1i:57:MET:O	41:1i:59:GLU:N	2.41	0.54
6:1G:99:PHE:HB2	6:1G:102:ARG:HH11	1.72	0.54
33:1a:264:C:O2'	49:1q:66:PRO:O	2.25	0.54
33:1a:1522:U:H5''	43:1k:128:ARG:HH22	1.72	0.54
1:1A:2351:G:O6	31:18:42:ARG:NH1	2.40	0.54
25:11:43:GLU:OE1	25:11:45:ARG:NH2	2.33	0.54
33:1a:126:G:OP1	33:1a:605:U:O2'	2.23	0.54
33:1a:483:C:O2	48:1p:13:LYS:NZ	2.41	0.54
34:1b:72:THR:HG23	34:1b:95:ARG:HA	1.90	0.54
45:1m:25:VAL:HG23	45:1m:29:ARG:HB3	1.90	0.54
21:1X:11:LEU:HD22	21:1X:32:LEU:HD13	1.90	0.54
46:1n:91:GLY:O	46:1n:93:ILE:N	2.41	0.54
1:1A:827:U:C2'	1:1A:2068:U:C2	2.85	0.54
1:1A:1184:U:OP2	27:13:31:ARG:NH2	2.41	0.54
9:1J:22:ALA:HA	9:1J:86:MET:HA	1.90	0.54
25:11:18:ARG:NH1	25:11:22:LEU:HB3	2.23	0.54
33:1a:350:G:OP1	52:1t:3:ASN:N	2.40	0.54
35:1c:156:ARG:NH1	35:1c:160:ALA:O	2.40	0.54
33:1a:1291:U:O2'	41:1i:42:GLU:OE2	2.23	0.53
42:1j:26:VAL:HG13	42:1j:36:VAL:HG11	1.90	0.53
44:1l:50:ARG:HG3	44:1l:90:LEU:HD11	1.90	0.53
1:1A:1817:G:H5''	3:1D:87:ARG:HG3	1.89	0.53
6:1G:73:SER:HB3	55:1x:67:C:O4'	2.08	0.53
11:1N:118:MET:HA	11:1N:121:LYS:HZ3	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1a:237:G:H4'	49:1q:27:ARG:NH1	2.21	0.53
46:1n:51:LEU:O	46:1n:53:ARG:N	2.41	0.53
1:1A:2267:A:H5''	1:1A:2268:A:H5'	1.90	0.53
1:1A:2485:G:H5''	14:1Q:45:GLN:HE21	1.73	0.53
16:1S:92:PHE:HE2	16:1S:94:ARG:HB3	1.74	0.53
39:1g:69:VAL:HG21	39:1g:104:ILE:HD11	1.89	0.53
41:1i:22:LYS:O	41:1i:62:ASP:N	2.40	0.53
52:1t:59:ASP:OD1	52:1t:76:LYS:NZ	2.29	0.53
53:1u:14:VAL:HG12	53:1u:16:LEU:H	1.74	0.53
23:1Z:55:GLU:HB3	23:1Z:59:GLU:CD	2.33	0.53
44:1l:3:THR:HG22	44:1l:5:ASN:H	1.73	0.53
48:1p:52:LEU:HD21	48:1p:57:ILE:HD12	1.90	0.53
1:1A:7:G:H5'	11:1N:132:HIS:CE1	2.44	0.53
7:1H:22:GLN:NE2	7:1H:38:ASN:O	2.42	0.53
24:10:65:GLY:HA2	24:10:85:GLU:HG3	1.90	0.53
1:1A:2037:A:H2'	1:1A:2038:G:C8	2.43	0.53
1:1A:2286:G:OP1	29:16:30:LYS:NZ	2.38	0.53
4:1E:2:ILE:HG13	4:1E:100:LEU:HD21	1.89	0.53
4:1E:49:GLN:HE21	4:1E:79:LEU:HB3	1.73	0.53
13:1P:85:VAL:HB	13:1P:94:THR:HG22	1.90	0.53
22:1Y:81:ASP:OD2	22:1Y:96:PHE:HB3	2.09	0.53
33:1a:675:A:H1'	43:1k:118:HIS:CE1	2.44	0.53
48:1p:42:ILE:O	48:1p:44:SER:N	2.42	0.53
1:1A:357:C:H2'	1:1A:358:U:C6	2.43	0.53
1:1A:1046:A:H4'	9:1J:58:THR:HG21	1.90	0.53
1:1A:2061:G:OP1	5:1F:63:LYS:NZ	2.35	0.53
4:1E:110:THR:HG21	4:1E:169:ARG:CZ	2.39	0.53
10:1K:33:VAL:HG22	10:1K:61:VAL:HG11	1.90	0.53
26:12:56:LEU:HA	26:12:59:GLU:HG2	1.90	0.53
29:16:10:LYS:HE3	29:16:53:LYS:O	2.08	0.53
30:17:34:ARG:HD2	30:17:42:LEU:HA	1.90	0.53
35:1c:22:TRP:HB3	35:1c:59:ARG:H	1.74	0.53
1:1A:1083:U:H4'	9:1J:42:ARG:NH1	2.18	0.53
15:1R:55:ALA:HA	15:1R:80:PHE:HE1	1.73	0.53
19:1V:73:LYS:NZ	19:1V:86:GLN:OE1	2.39	0.53
37:1e:154:ALA:HA	37:1e:157:ARG:HB3	1.91	0.53
1:1A:142:A:H2'	1:1A:143:C:C6	2.44	0.53
1:1A:1478:G:H1	1:1A:1513:U:H3	1.56	0.53
22:1Y:33:LYS:HE2	22:1Y:66:GLN:NE2	2.24	0.53
26:12:26:PHE:HD1	26:12:29:ARG:HH11	1.55	0.53
33:1a:409:U:H3	33:1a:433:G:H1	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1l:29:GLN:HB3	44:1l:81:LEU:HD11	1.91	0.53
49:1q:24:ALA:HA	49:1q:43:LYS:HA	1.91	0.53
1:1A:1171:G:C4	1:1A:1172:C:N4	2.76	0.52
7:1H:4:VAL:O	7:1H:69:ARG:HG2	2.09	0.52
10:1K:8:TYR:CE1	10:1K:60:THR:HG23	2.44	0.52
10:1K:79:LEU:HD23	10:1K:82:LYS:HD3	1.91	0.52
8:1I:90:LEU:HD11	8:1I:146:VAL:HG11	1.91	0.52
28:15:27:SER:O	28:15:40:ARG:HG3	2.09	0.52
33:1a:780:A:N6	33:1a:801:U:OP2	2.42	0.52
33:1a:1363:A:O2'	33:1a:1365:G:N7	2.38	0.52
43:1k:35:THR:HA	43:1k:42:LEU:H	1.74	0.52
1:1A:17:G:H4'	18:1U:25:TYR:HE1	1.74	0.52
6:1G:103:LEU:HA	6:1G:107:ALA:HB3	1.91	0.52
17:1T:30:VAL:HG13	17:1T:80:VAL:HG12	1.91	0.52
33:1a:429:U:H5'	36:1d:9:LEU:HD23	1.92	0.52
33:1a:1437:A:H5''	52:1t:29:ARG:HH12	1.75	0.52
55:1x:8:U:O3'	55:1x:22:G:N2	2.41	0.52
1:1A:995:C:O2	11:1N:3:THR:OG1	2.20	0.52
1:1A:1140:C:OP2	11:1N:68:LYS:NZ	2.36	0.52
1:1A:1266:G:O2'	1:1A:2012:G:O6	2.25	0.52
11:1N:135:GLN:N	11:1N:135:GLN:OE1	2.43	0.52
15:1R:55:ALA:HA	15:1R:80:PHE:CD1	2.44	0.52
33:1a:553:A:H5''	44:1l:21:VAL:HG21	1.90	0.52
33:1a:977:A:OP1	46:1n:61:ARG:NH2	2.42	0.52
34:1b:128:LYS:HG3	34:1b:129:LEU:HG	1.91	0.52
14:1Q:50:ARG:HA	14:1Q:53:MET:CG	2.39	0.52
33:1a:1397:C:P	37:1e:29:ARG:HH22	2.33	0.52
1:1A:448:U:O4'	5:1F:79:ARG:NE	2.41	0.52
1:1A:827:U:H2'	1:1A:2068:U:N3	2.24	0.52
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.44	0.52
33:1a:96:U:H2'	33:1a:97:G:C8	2.45	0.52
42:1j:78:GLU:OE2	42:1j:80:THR:OG1	2.27	0.52
52:1t:73:ALA:HA	52:1t:76:LYS:HG2	1.91	0.52
1:1A:1216:G:H5''	18:1U:11:ARG:HH12	1.74	0.52
3:1D:2:ALA:N	3:1D:20:VAL:O	2.43	0.52
4:1E:14:ILE:HA	17:1T:12:GLN:HE22	1.75	0.52
9:1J:57:ASN:ND2	9:1J:78:GLY:O	2.27	0.52
11:1N:114:LEU:HG	11:1N:118:MET:HE3	1.92	0.52
28:15:13:ARG:HG3	28:15:16:ARG:NH1	2.22	0.52
30:17:12:ARG:HG2	30:17:12:ARG:HH21	1.75	0.52
33:1a:1064:G:O2'	33:1a:1190:G:N2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1a:1151:A:O2'	33:1a:1152:A:H5''	2.10	0.52
39:1g:72:THR:HA	39:1g:96:ARG:HH12	1.75	0.52
1:1A:139:U:O4	21:1X:2:ILE:HG13	2.10	0.52
1:1A:1667:G:O2'	1:1A:1991:U:O4	2.25	0.52
10:1K:98:VAL:HG23	10:1K:138:LEU:HD23	1.91	0.52
27:13:28:GLY:HA3	27:13:38:ARG:HH21	1.75	0.52
31:18:9:GLY:O	31:18:13:ARG:NH2	2.43	0.52
33:1a:677:U:H3	33:1a:713:G:H22	1.58	0.52
33:1a:1152:A:OP1	42:1j:70:HIS:ND1	2.43	0.52
33:1a:1380:U:O2'	39:1g:3:ARG:NH1	2.43	0.52
35:1c:11:ARG:NH2	35:1c:177:THR:O	2.43	0.52
41:1i:118:LEU:HG	41:1i:124:ARG:HA	1.92	0.52
46:1n:52:PRO:O	46:1n:54:ASP:N	2.34	0.52
1:1A:581:C:H2'	1:1A:582:A:C8	2.45	0.52
33:1a:409:U:OP2	36:1d:22:LYS:NZ	2.32	0.52
34:1b:146:ASN:OD1	34:1b:147:SER:N	2.43	0.52
36:1d:145:ILE:HD13	36:1d:178:MET:HB3	1.92	0.52
7:1H:98:VAL:HG22	7:1H:103:ILE:HG12	1.90	0.51
8:1I:127:GLU:HG2	8:1I:145:ASN:HD22	1.74	0.51
31:18:16:LYS:HA	31:18:22:PHE:HD1	1.75	0.51
1:1A:1223:G:N2	1:1A:1226:A:OP2	2.43	0.51
8:1I:113:SER:O	8:1I:116:ARG:NH1	2.41	0.51
33:1a:982:U:H4'	33:1a:983:A:H5'	1.92	0.51
40:1h:106:THR:OG1	40:1h:109:GLY:O	2.25	0.51
1:1A:137:U:H3	1:1A:142:A:H61	1.57	0.51
5:1F:61:ARG:HE	5:1F:65:THR:HG23	1.76	0.51
13:1P:63:LYS:O	31:18:30:ARG:NH1	2.41	0.51
36:1d:83:LYS:O	36:1d:89:ASN:ND2	2.42	0.51
24:10:37:ILE:HD11	24:10:82:ILE:HD11	1.93	0.51
29:16:6:ARG:NH2	29:16:26:ASN:HB2	2.22	0.51
36:1d:12:SER:HB3	36:1d:18:ASP:HA	1.93	0.51
55:1x:7:G:N2	55:1x:78:C:O2	2.43	0.51
1:1A:2886[B]:A:H3'	1:1A:2887[B]:A:C5'	2.41	0.51
8:1I:21:VAL:HG21	8:1I:25:TYR:HD2	1.76	0.51
33:1a:923:A:N6	33:1a:1392:G:O6	2.43	0.51
40:1h:66:PHE:CD2	40:1h:67:GLN:HG2	2.45	0.51
1:1A:1651:G:OP1	15:1R:40:LYS:NZ	2.43	0.51
4:1E:46:ARG:NH2	4:1E:88:GLU:O	2.38	0.51
20:1W:83:LYS:O	20:1W:84:ARG:NH2	2.38	0.51
38:1f:62:MET:HG2	38:1f:64:VAL:HG23	1.91	0.51
41:1i:28:ILE:HG23	41:1i:63:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.46	0.51
6:1G:25:VAL:O	6:1G:28:VAL:HG12	2.11	0.51
34:1b:70:VAL:HB	34:1b:163:VAL:HA	1.92	0.51
40:1h:13:ARG:HB3	40:1h:25:VAL:HG11	1.93	0.51
42:1j:12:ALA:HB3	42:1j:18:ILE:HB	1.93	0.51
45:1m:5:ALA:H	45:1m:57:ARG:NH1	2.09	0.51
1:1A:137:U:H3	1:1A:142:A:N6	2.09	0.51
1:1A:1597:A:H5''	1:1A:1598:A:H5'	1.93	0.51
1:1A:1824:G:H5''	3:1D:52:ARG:NH1	2.25	0.51
1:1A:2162:G:H5''	1:1A:2171:A:H2'	1.93	0.51
33:1a:954:G:H21	33:1a:1227:A:H61	1.59	0.51
1:1A:1869:G:N2	1:1A:1871:A:O2'	2.43	0.51
1:1A:2321:U:H5'	1:1A:2322:A:OP2	2.11	0.51
1:1A:2882:A:P	15:1R:96:ARG:HE	2.34	0.51
3:1D:130:LEU:HD11	3:1D:135:ILE:HG13	1.92	0.51
33:1a:403:C:H5'	36:1d:132:ILE:HG23	1.92	0.51
33:1a:1105:A:H2'	33:1a:1106:G:C8	2.46	0.51
49:1q:70:THR:HG22	49:1q:71:LYS:H	1.76	0.51
1:1A:572:A:OP2	19:1V:79:ARG:NH1	2.44	0.51
1:1A:639:U:H2'	1:1A:640:C:C6	2.46	0.51
1:1A:1026:G:H2'	1:1A:1027:A:C8	2.46	0.51
1:1A:2000:C:OP1	15:1R:5:LYS:NZ	2.39	0.51
13:1P:109:LYS:HG2	13:1P:126:ARG:HB2	1.92	0.51
33:1a:522:C:OP2	44:1l:66:TYR:OH	2.23	0.51
37:1e:15:LEU:HA	37:1e:37:THR:HG22	1.92	0.51
1:1A:112:U:H5'	26:12:58:ASN:ND2	2.26	0.50
1:1A:748:G:OP1	20:1W:88:ARG:NH1	2.43	0.50
1:1A:1799:G:H8	3:1D:180:GLU:OE1	1.93	0.50
1:1A:2874:C:H5''	15:1R:4:ARG:HH21	1.76	0.50
4:1E:152:PRO:HG3	4:1E:156:PHE:CZ	2.46	0.50
33:1a:1414:U:H2'	33:1a:1415:G:H8	1.75	0.50
1:1A:729:G:C6	3:1D:207:LYS:HB2	2.47	0.50
3:1D:58:HIS:ND1	3:1D:59:LYS:O	2.35	0.50
34:1b:193:PRO:O	34:1b:195:GLY:N	2.41	0.50
35:1c:84:VAL:HG13	35:1c:101:ILE:HD13	1.93	0.50
39:1g:27:VAL:HG12	39:1g:43:VAL:HG21	1.93	0.50
44:1l:22:PRO:O	44:1l:24:LEU:N	2.40	0.50
1:1A:827:U:C2'	1:1A:2068:U:O2	2.58	0.50
1:1A:2116:G:N7	1:1A:2165:C:N4	2.58	0.50
24:10:46:HIS:HB2	24:10:79:PHE:CD1	2.45	0.50
35:1c:180:ALA:HB1	35:1c:203:PHE:HE1	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2313:C:O4'	6:1G:37:ASN:ND2	2.44	0.50
1:1A:2784:U:H4'	4:1E:43:ASP:OD1	2.10	0.50
4:1E:152:PRO:HG3	4:1E:156:PHE:CE1	2.46	0.50
13:1P:23:ILE:HG12	19:1V:82:HIS:HD2	1.75	0.50
14:1Q:49:ALA:HB1	14:1Q:120:ALA:HB1	1.92	0.50
16:1S:37:ALA:HB3	16:1S:78:VAL:HG11	1.94	0.50
19:1V:68:ARG:NH1	19:1V:90:ARG:HB2	2.26	0.50
29:16:5:ILE:HG21	29:16:28:ARG:HE	1.76	0.50
33:1a:199:A:H2'	33:1a:200:G:C8	2.46	0.50
36:1d:62:ARG:O	36:1d:66:GLY:N	2.41	0.50
1:1A:536:G:H4'	18:1U:57:PHE:HZ	1.76	0.50
1:1A:1847:G:O5'	1:1A:1847:G:H8	1.95	0.50
7:1H:52:PHE:CZ	7:1H:72:LEU:HD22	2.47	0.50
13:1P:57:LEU:HG	31:18:14:PHE:HZ	1.77	0.50
31:18:39:LYS:HA	31:18:42:ARG:NH2	2.25	0.50
33:1a:412:A:O2'	33:1a:413:G:H4'	2.12	0.50
35:1c:56:VAL:HB	35:1c:67:THR:HB	1.92	0.50
45:1m:106:ALA:O	45:1m:110:LYS:HB3	2.11	0.50
33:1a:426:U:OP2	36:1d:33:LYS:NZ	2.45	0.50
33:1a:1166:G:H2'	33:1a:1168:U:OP2	2.12	0.50
1:1A:2086:U:H2'	1:1A:2087:G:C8	2.46	0.50
1:1A:2428:G:N2	13:1P:54:GLN:HE21	2.10	0.50
10:1K:18:ALA:C	10:1K:20:PRO:HD3	2.37	0.50
10:1K:54:PRO:HD2	10:1K:78:VAL:HG11	1.94	0.50
1:1A:84:A:N1	1:1A:98:G:O2'	2.38	0.50
1:1A:851:C:H2'	1:1A:852:U:C6	2.47	0.50
1:1A:2020:A:H5'	28:15:9:THR:CG2	2.42	0.50
6:1G:13:VAL:O	6:1G:17:MET:HG2	2.12	0.50
48:1p:4:ILE:HG13	48:1p:21:VAL:HG22	1.93	0.50
1:1A:483:A:C4	22:1Y:58:ILE:HD11	2.47	0.50
9:1J:21:GLY:HA3	9:1J:86:MET:CE	2.42	0.50
9:1J:88:HIS:ND1	9:1J:89:PRO:O	2.45	0.50
26:12:39:GLN:HB3	26:12:41:HIS:CE1	2.47	0.50
29:16:25:LYS:HE2	29:16:30:LYS:O	2.11	0.50
1:1A:2291:U:H2'	1:1A:2292:U:C6	2.47	0.49
23:1Z:1:MET:HE3	23:1Z:62:THR:HG23	1.94	0.49
33:1a:1373:G:H5''	39:1g:36:LYS:HE2	1.93	0.49
37:1e:88:VAL:HG12	37:1e:93:ARG:HG2	1.93	0.49
41:1i:129:LYS:HG3	41:1i:130:ARG:H	1.77	0.49
1:1A:395:U:O2'	1:1A:396:G:N7	2.39	0.49
10:1K:20:PRO:HB2	10:1K:23:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1N:72:LYS:HE3	11:1N:74:TYR:CE1	2.46	0.49
33:1a:177:G:H5'	52:1t:60:ARG:NH1	2.27	0.49
33:1a:375:U:O2	48:1p:28:ARG:NH2	2.45	0.49
1:1A:142:A:C5	1:1A:143:C:C4	3.00	0.49
33:1a:689:C:HO2'	33:1a:705:G:HO2'	1.56	0.49
33:1a:1013:G:N2	33:1a:1016:A:OP2	2.45	0.49
38:1f:36:ILE:HG13	38:1f:64:VAL:HG22	1.95	0.49
1:1A:857:G:H5'	24:10:69:PHE:CD2	2.48	0.49
38:1f:50:PRO:HG3	38:1f:55:HIS:CE1	2.47	0.49
42:1j:65:TYR:HB3	46:1n:96:LEU:HD11	1.93	0.49
1:1A:245:G:N7	31:18:8:ARG:NH2	2.55	0.49
1:1A:1028:A:N6	1:1A:1125:G:H2'	2.28	0.49
10:1K:59:ILE:HD11	10:1K:67:PHE:CD1	2.47	0.49
18:1U:108:ALA:O	18:1U:112:LYS:HG2	2.12	0.49
43:1k:127:ARG:HB2	53:1u:34:ARG:HE	1.77	0.49
1:1A:1832:C:H5''	33:1a:900:A:H4'	1.93	0.49
11:1N:7:LYS:O	11:1N:11:VAL:HG23	2.12	0.49
18:1U:105:ALA:HB1	19:1V:40:MET:HE1	1.95	0.49
24:10:45:PHE:HE1	24:10:78:LYS:HD3	1.76	0.49
33:1a:658:C:H1'	47:1o:22:THR:HG21	1.94	0.49
39:1g:111:ARG:O	39:1g:119:ARG:NH2	2.45	0.49
1:1A:929:U:H4'	27:13:38:ARG:NH2	2.27	0.49
18:1U:49:ASP:HA	18:1U:52:GLN:HB2	1.94	0.49
43:1k:124:PRO:HB2	43:1k:126:LYS:HG2	1.94	0.49
1:1A:781:A:P	3:1D:217:ARG:HH22	2.36	0.49
1:1A:1656:C:OP1	4:1E:141:ARG:NE	2.41	0.49
6:1G:73:SER:HB3	6:1G:80:ARG:HA	1.94	0.49
8:1I:21:VAL:CG2	8:1I:25:TYR:HD2	2.25	0.49
14:1Q:10:ARG:HH22	14:1Q:11:LYS:HE3	1.77	0.49
33:1a:1222:G:OP2	33:1a:1322:C:N4	2.46	0.49
41:1i:7:TYR:HD1	41:1i:20:PHE:HE1	1.59	0.49
50:1r:57:ARG:HE	50:1r:61:ARG:HH21	1.59	0.49
1:1A:551:G:H5'	1:1A:551:G:H8	1.78	0.49
1:1A:1059:G:O2'	10:1K:117:MET:HE1	2.13	0.49
33:1a:115:G:H4'	33:1a:116:A:O5'	2.11	0.49
34:1b:85:LEU:HD13	34:1b:91:PHE:HE2	1.78	0.49
1:1A:1656:C:P	4:1E:141:ARG:HE	2.36	0.49
1:1A:2547:A:H2'	1:1A:2548:U:C6	2.48	0.49
1:1A:2547:A:H4'	12:1O:29:HIS:CE1	2.47	0.49
2:1B:66:A:H61	2:1B:107:G:H2'	1.77	0.49
20:1W:82:MET:HB2	20:1W:98:LYS:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:16:35:GLU:OE2	29:16:48:ILE:HD11	2.13	0.49
33:1a:713:G:H2'	33:1a:714:G:C8	2.48	0.49
33:1a:1414:U:H2'	33:1a:1415:G:C8	2.47	0.49
39:1g:116:MET:HA	39:1g:119:ARG:HD3	1.94	0.49
1:1A:281:C:H2'	1:1A:282:A:C8	2.48	0.48
1:1A:2831:G:P	4:1E:56:LYS:HE2	2.53	0.48
14:1Q:10:ARG:NH2	14:1Q:11:LYS:HE3	2.28	0.48
15:1R:8:ARG:NH2	15:1R:39:PRO:HA	2.27	0.48
17:1T:86:VAL:HG11	17:1T:89:ARG:HG2	1.94	0.48
33:1a:176:C:H4'	52:1t:24:ARG:HH21	1.77	0.48
33:1a:1072:G:O6	33:1a:1102:A:N6	2.46	0.48
41:1i:99:ARG:NH1	41:1i:105:THR:OG1	2.44	0.48
1:1A:2067:G:O2'	1:1A:2069:G7M:H5''	2.14	0.48
6:1G:75:ALA:HB2	55:1x:68:A:H5'	1.95	0.48
9:1J:33:VAL:HG21	9:1J:106:PHE:CE2	2.47	0.48
12:1O:30:ARG:NH2	12:1O:37:ASP:OD2	2.46	0.48
31:18:42:ARG:HG3	31:18:45:ARG:NH2	2.28	0.48
33:1a:111:G:O2'	33:1a:389:A:O2'	2.29	0.48
33:1a:202:G:H1	33:1a:215:C:H42	1.59	0.48
33:1a:1359:C:H3'	46:1n:75:ARG:HH22	1.78	0.48
33:1a:1437:A:H2'	33:1a:1438:G:H8	1.78	0.48
9:1J:72:LEU:HD21	9:1J:112:ALA:HB2	1.95	0.48
22:1Y:85:PHE:CE1	22:1Y:94:ARG:HG2	2.45	0.48
33:1a:560:A:H4'	33:1a:561:U:H5''	1.95	0.48
1:1A:337:C:OP2	22:1Y:4:LYS:NZ	2.39	0.48
1:1A:479:A:N3	1:1A:481:G:H5''	2.28	0.48
1:1A:781:A:OP1	3:1D:217:ARG:NH2	2.46	0.48
2:1B:48:U:H4'	16:1S:100:HIS:HD2	1.78	0.48
6:1G:67:ILE:HA	6:1G:87:CYS:HA	1.93	0.48
11:1N:110:PRO:O	11:1N:115:GLY:HA3	2.13	0.48
23:1Z:76:ASP:OD1	23:1Z:77:VAL:N	2.45	0.48
25:11:12:PRO:CB	25:11:28:ARG:HH21	2.26	0.48
33:1a:147:G:H2'	33:1a:148:G:C8	2.49	0.48
35:1c:138:VAL:HA	35:1c:149:ILE:HD13	1.94	0.48
36:1d:70:ARG:O	36:1d:74:ASN:ND2	2.46	0.48
1:1A:1172:C:C4	1:1A:1173:U:H1'	2.48	0.48
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.29	0.48
1:1A:2079:U:O2'	25:11:23:ASN:OD1	2.30	0.48
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.29	0.48
1:1A:2845:U:H5''	17:1T:52:ASN:O	2.14	0.48
4:1E:5:VAL:HG11	4:1E:80:TRP:CZ3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1T:106:LYS:HG2	33:1a:1432:G:O5'	2.13	0.48
36:1d:50:ASP:O	36:1d:54:GLN:HG2	2.13	0.48
49:1q:27:ARG:HH21	49:1q:40:ARG:HG2	1.79	0.48
1:1A:1412:U:H2'	1:1A:1413:A:C8	2.49	0.48
1:1A:2451:A:N3	55:1x:87:A:O2'	2.46	0.48
6:1G:5:HIS:NE2	6:1G:9:LYS:HE3	2.28	0.48
6:1G:69:LYS:HE3	6:1G:84:PRO:HG3	1.96	0.48
9:1J:21:GLY:CA	9:1J:86:MET:CE	2.88	0.48
33:1a:1072:G:OP1	37:1e:62:LYS:NZ	2.45	0.48
41:1i:17:ALA:HB2	41:1i:67:VAL:HG23	1.96	0.48
48:1p:4:ILE:HG22	48:1p:71:VAL:HG21	1.95	0.48
48:1p:23:ASP:OD2	48:1p:25:ARG:NH1	2.46	0.48
1:1A:355:U:H2'	1:1A:356:G:C8	2.49	0.48
1:1A:674:G:HI'	5:1F:69:ARG:NE	2.20	0.48
23:1Z:63:ILE:HG22	23:1Z:65:VAL:HG23	1.95	0.48
33:1a:875:U:O3'	40:1h:15:ARG:NH1	2.47	0.48
39:1g:69:VAL:HA	39:1g:138:ARG:HD3	1.95	0.48
1:1A:1040:A:OP1	23:1Z:46:LYS:NZ	2.47	0.48
1:1A:1847:G:N2	1:1A:1848:A:N6	2.37	0.48
33:1a:589:U:H3	33:1a:650:G:H1	1.60	0.48
33:1a:1360:A:OP2	46:1n:75:ARG:NH2	2.47	0.48
34:1b:94:HIS:CG	34:1b:146:ASN:HB2	2.48	0.48
1:1A:906:U:O2'	14:1Q:66:ARG:NH2	2.29	0.47
1:1A:906:U:HO2'	14:1Q:66:ARG:HH21	1.58	0.47
10:1K:12:GLN:HA	10:1K:56:PRO:HA	1.95	0.47
10:1K:61:VAL:HG12	10:1K:67:PHE:HB3	1.96	0.47
17:1T:89:ARG:HB3	17:1T:113:ARG:HH12	1.78	0.47
33:1a:252:U:O4	33:1a:253:A:N6	2.44	0.47
33:1a:587:G:N2	33:1a:754:C:OP2	2.35	0.47
33:1a:978:A:OP2	33:1a:1362:A:N6	2.47	0.47
35:1c:20:SER:HB3	35:1c:22:TRP:NE1	2.29	0.47
1:1A:323:C:H2'	5:1F:163:ASN:OD1	2.14	0.47
1:1A:594:U:H2'	1:1A:595:C:C6	2.48	0.47
3:1D:243:HIS:O	3:1D:245:VAL:HG13	2.14	0.47
9:1J:33:VAL:HG22	9:1J:105:LYS:HE2	1.97	0.47
11:1N:102:GLU:HG3	11:1N:124:VAL:HG21	1.97	0.47
14:1Q:34:LYS:HE3	14:1Q:131:VAL:HG11	1.95	0.47
16:1S:35:ILE:HD12	16:1S:102:ARG:HG2	1.96	0.47
19:1V:1:MET:HE3	19:1V:101:ILE:HB	1.96	0.47
35:1c:79:LYS:O	35:1c:81:GLY:N	2.47	0.47
35:1c:189:ALA:HB3	35:1c:196:ILE:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:1j:52:LEU:HD23	42:1j:62:ARG:HG2	1.96	0.47
33:1a:890:G:O2'	33:1a:906:A:N6	2.47	0.47
33:1a:1265:C:N4	33:1a:1266:G:O6	2.47	0.47
45:1m:114:LYS:H	45:1m:115:PRO:HD2	1.78	0.47
3:1D:71:LYS:NZ	3:1D:98:ASP:OD2	2.37	0.47
6:1G:78:LYS:NZ	55:1x:68:A:O2'	2.46	0.47
9:1J:18:VAL:O	9:1J:86:MET:SD	2.72	0.47
11:1N:140:LEU:HG	11:1N:142:ILE:HB	1.96	0.47
18:1U:44:GLN:NE2	19:1V:77:PHE:HB3	2.18	0.47
33:1a:950:U:H2'	33:1a:951:G:C8	2.49	0.47
33:1a:1477:U:H2'	33:1a:1478:U:C6	2.49	0.47
33:1a:1516:G:N2	33:1a:1519:A:OP2	2.47	0.47
34:1b:173:ILE:HG23	34:1b:183:VAL:HG11	1.95	0.47
1:1A:1047:G:HO2'	1:1A:1110:G:H1	1.63	0.47
18:1U:67:ALA:O	18:1U:71:GLN:HG2	2.14	0.47
38:1f:10:VAL:HB	38:1f:58:HIS:HB3	1.96	0.47
1:1A:832:U:H2'	1:1A:833:A:C8	2.49	0.47
1:1A:1827:U:OP2	3:1D:221:ARG:NH1	2.47	0.47
1:1A:2362:C:H5''	31:18:40:ARG:NH1	2.29	0.47
6:1G:71:ARG:HG2	6:1G:72:LYS:HG2	1.97	0.47
7:1H:43:VAL:HG23	7:1H:52:PHE:HE1	1.80	0.47
20:1W:48:LYS:HE2	20:1W:52:GLU:OE2	2.15	0.47
33:1a:410:G:H2'	33:1a:429:U:C4	2.50	0.47
34:1b:117:LEU:HB3	34:1b:141:LEU:HD11	1.95	0.47
35:1c:168:TYR:OH	37:1e:55:GLU:OE2	2.19	0.47
35:1c:185:ASN:OD1	35:1c:186:THR:N	2.42	0.47
36:1d:168:PRO:HB3	36:1d:170:TRP:CH2	2.49	0.47
51:1s:53:ASN:HB3	51:1s:75:ALA:HB1	1.97	0.47
1:1A:340:A:O2'	5:1F:162:ARG:NH1	2.47	0.47
1:1A:494:G:H4'	20:1W:6:LYS:HB2	1.95	0.47
1:1A:644:A:H2'	1:1A:645:C:O4'	2.15	0.47
1:1A:1868:C:H2'	1:1A:1869:G:O4'	2.13	0.47
1:1A:1902:C:H5''	3:1D:240:PHE:CE2	2.49	0.47
1:1A:2189:U:H2'	1:1A:2190:G:O4'	2.15	0.47
1:1A:2886[B]:A:H3'	1:1A:2887[B]:A:H5'	1.96	0.47
10:1K:79:LEU:HA	10:1K:82:LYS:HG2	1.95	0.47
14:1Q:76:LYS:NZ	14:1Q:85:GLY:O	2.46	0.47
16:1S:17:LYS:HA	16:1S:20:GLU:OE2	2.14	0.47
30:17:16:HIS:HA	30:17:21:ARG:NH2	2.28	0.47
33:1a:426:U:H4'	36:1d:40:GLN:HA	1.97	0.47
34:1b:166:ALA:HB2	34:1b:187:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:1j:35:GLN:HB3	42:1j:77:VAL:HB	1.96	0.47
43:1k:31:ILE:HG13	43:1k:46:THR:HG22	1.95	0.47
51:1s:50:ALA:HA	51:1s:59:PRO:HA	1.97	0.47
1:1A:2233:U:H2'	1:1A:2234:G:C8	2.50	0.47
1:1A:2386:A:N3	24:10:41[A]:ARG:HG3	2.30	0.47
1:1A:2461:A:H1'	1:1A:2492:U:C2	2.50	0.47
1:1A:2812:G:H2'	1:1A:2813:A:O4'	2.15	0.47
1:1A:2874:C:OP1	15:1R:4:ARG:NH2	2.48	0.47
4:1E:4:LEU:HD22	4:1E:32:ASN:HD22	1.80	0.47
5:1F:70:SER:HB2	5:1F:78:TRP:CH2	2.50	0.47
16:1S:92:PHE:CE2	16:1S:94:ARG:HB3	2.50	0.47
23:1Z:70:ILE:HG22	23:1Z:72:VAL:HG13	1.97	0.47
43:1k:29:ASN:HB2	43:1k:57:LYS:NZ	2.30	0.47
1:1A:572:A:H5'	19:1V:79:ARG:NH2	2.30	0.47
1:1A:2602:A:C8	55:1x:86:C:OP2	2.67	0.47
11:1N:69:ARG:O	11:1N:90:GLU:HB2	2.13	0.47
29:16:21:TYR:CD2	29:16:38:LYS:HD3	2.49	0.47
33:1a:1125:U:H4'	42:1j:7:ARG:NH1	2.26	0.47
42:1j:9:ARG:NH2	42:1j:99:GLN:OE1	2.47	0.47
43:1k:26:SER:OG	43:1k:29:ASN:O	2.26	0.47
1:1A:2091:C:O2'	25:11:56:MET:HE1	2.15	0.47
1:1A:2888[A]:C:H2'	1:1A:2889:C:C6	2.50	0.47
15:1R:63:ARG:HA	15:1R:80:PHE:HE2	1.80	0.47
33:1a:972:C:H4'	42:1j:59:LYS:HD3	1.97	0.47
33:1a:1221:G:H4'	51:1s:77:THR:HG21	1.97	0.47
37:1e:105:ILE:HD13	37:1e:121:HIS:HA	1.97	0.47
52:1t:15:GLU:OE2	52:1t:18:ARG:NH2	2.34	0.47
1:1A:289:G:H2'	1:1A:290:U:O4'	2.15	0.46
1:1A:2529:G:H4'	7:1H:175:LYS:HG3	1.97	0.46
1:1A:2615:U:C2	28:15:4:GLN:HA	2.50	0.46
56:1A:3001:6UQ:CLAG	14:1Q:54:THR:HG22	2.53	0.46
4:1E:13:ARG:HH11	17:1T:56:HIS:HA	1.79	0.46
4:1E:35:THR:HG22	4:1E:73:VAL:HG21	1.98	0.46
5:1F:29:HIS:CE1	5:1F:33:VAL:HG21	2.51	0.46
7:1H:11:VAL:HG21	7:1H:17:VAL:HG23	1.97	0.46
31:18:26:HIS:CE1	31:18:48:ALA:HB2	2.49	0.46
33:1a:96:U:H2'	33:1a:97:G:H8	1.79	0.46
33:1a:1051:C:H42	33:1a:1207:G:H1	1.63	0.46
36:1d:85:ASN:OD1	37:1e:103:THR:OG1	2.25	0.46
1:1A:323:C:HO2'	1:1A:1205:A:H61	1.60	0.46
4:1E:13:ARG:HG2	17:1T:56:HIS:HE1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:147:ASP:OD1	6:1G:150:ARG:NH1	2.32	0.46
33:1a:362:G:OP2	44:1l:31:ARG:NH2	2.45	0.46
33:1a:543:U:OP1	36:1d:14:ARG:NE	2.48	0.46
43:1k:29:ASN:HB2	43:1k:57:LYS:HZ3	1.80	0.46
44:1l:30:LYS:O	44:1l:82:ILE:HG22	2.14	0.46
1:1A:65:U:O3'	21:1X:73:ARG:NH1	2.43	0.46
4:1E:14:ILE:HD13	17:1T:12:GLN:HE22	1.81	0.46
11:1N:26:GLY:O	11:1N:30:THR:HG23	2.15	0.46
33:1a:1227:A:H5'	45:1m:110:LYS:NZ	2.30	0.46
48:1p:12:LYS:HG2	48:1p:13:LYS:HG2	1.96	0.46
1:1A:2019:A:H4'	18:1U:34:VAL:HG21	1.97	0.46
9:1J:29:ASP:OD1	9:1J:30:SER:N	2.49	0.46
12:1O:20:MET:HE3	12:1O:22:ILE:HG22	1.96	0.46
13:1P:110:VAL:HG11	13:1P:135:ILE:HD11	1.98	0.46
24:10:38:VAL:HG12	24:10:59:LEU:HB2	1.97	0.46
33:1a:206:C:N4	33:1a:213:G:H1	2.13	0.46
33:1a:427:U:OP2	33:1a:428:G:O2'	2.25	0.46
33:1a:1516:G:H2'	33:1a:1518:A:OP2	2.15	0.46
46:1n:3:LYS:HD2	46:1n:6:MET:HG2	1.97	0.46
49:1q:48:ASP:HB3	49:1q:75:LEU:HD21	1.97	0.46
1:1A:1183:U:H2'	1:1A:1184:U:C6	2.51	0.46
5:1F:49:ARG:HH11	5:1F:72:SER:HB3	1.80	0.46
14:1Q:50:ARG:HA	14:1Q:53:MET:HG3	1.98	0.46
18:1U:36:PHE:HZ	19:1V:84:ARG:NH2	2.13	0.46
28:15:53:LYS:HE3	28:15:56:ALA:HA	1.98	0.46
35:1c:20:SER:HB3	35:1c:22:TRP:CD1	2.51	0.46
41:1i:106:ARG:NH1	41:1i:107:ASP:O	2.49	0.46
10:1K:59:ILE:HD12	10:1K:69:PHE:HB3	1.97	0.46
30:17:34:ARG:HG2	30:17:42:LEU:HD23	1.98	0.46
33:1a:816:A:OP1	33:1a:1526:G:O2'	2.28	0.46
35:1c:59:ARG:HE	35:1c:64:ILE:HD12	1.80	0.46
38:1f:41:ASP:OD1	38:1f:58:HIS:NE2	2.46	0.46
1:1A:1919:A:H2	33:1a:1496:C:O4'	1.98	0.46
1:1A:2054:A:H2'	28:15:5:GLN:HE22	1.81	0.46
1:1A:2813:A:H2	1:1A:2887[B]:A:N6	2.11	0.46
3:1D:30:PHE:HB3	3:1D:103:TYR:OH	2.16	0.46
3:1D:130:LEU:HD13	3:1D:134:ASN:HB2	1.97	0.46
5:1F:23:PHE:HB2	5:1F:111:GLU:OE2	2.15	0.46
6:1G:38:MET:HE3	6:1G:152:LEU:HD12	1.98	0.46
14:1Q:30:SER:H	14:1Q:106:ASP:HB3	1.79	0.46
14:1Q:42:THR:HG22	14:1Q:93:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1S:1:MET:SD	16:1S:6:ALA:HA	2.56	0.46
17:1T:106:LYS:HA	17:1T:109:ARG:NH2	2.31	0.46
33:1a:718:A:H5'	43:1k:119:ASN:ND2	2.31	0.46
33:1a:1319:A:OP2	51:1s:5:LEU:HD11	2.15	0.46
40:1h:95:VAL:HG23	40:1h:102:ALA:HB2	1.97	0.46
40:1h:103:VAL:HG12	40:1h:126:ILE:HD13	1.97	0.46
42:1j:15:HIS:CD2	42:1j:16:ARG:HG3	2.51	0.46
1:1A:588:U:H1'	5:1F:85:PHE:CD1	2.51	0.46
1:1A:2485:G:H5''	14:1Q:45:GLN:NE2	2.31	0.46
10:1K:22:PRO:HB2	10:1K:23:PRO:HD3	1.97	0.46
11:1N:49:ASP:HB2	11:1N:114:LEU:HD11	1.98	0.46
33:1a:19:A:OP1	37:1e:135:ASN:ND2	2.49	0.46
33:1a:784:A:H2'	33:1a:785:G:C8	2.50	0.46
35:1c:191:THR:OG1	35:1c:194:GLY:O	2.33	0.46
36:1d:95:GLU:HA	36:1d:100:ASN:ND2	2.29	0.46
1:1A:1007:C:OP1	11:1N:37:ARG:NH2	2.49	0.46
1:1A:1715:G:O2'	1:1A:1743:G:O6	2.32	0.46
12:1O:1:MET:HE3	12:1O:32:TYR:CE2	2.51	0.46
14:1Q:63:ILE:HG12	14:1Q:105:MET:HE2	1.96	0.46
15:1R:32:GLU:HB3	15:1R:118:ARG:HG3	1.98	0.46
33:1a:626:G:OP1	48:1p:35:ARG:NH2	2.45	0.46
33:1a:1367:C:H5'	42:1j:62:ARG:NH1	2.31	0.46
51:1s:63:THR:HG22	51:1s:64:ASP:H	1.81	0.46
52:1t:51:PHE:HA	52:1t:54:MET:HG2	1.97	0.46
1:1A:1171:G:H2'	1:1A:1172:C:C5	2.50	0.46
3:1D:131:PRO:HG3	3:1D:189:ARG:NE	2.31	0.46
12:1O:4:GLU:O	12:1O:5:GLN:HB2	2.16	0.46
23:1Z:24:ASN:OD1	23:1Z:44:HIS:HB3	2.16	0.46
17:1T:27:GLU:OE1	17:1T:87:LYS:HE3	2.17	0.45
23:1Z:21:ARG:HA	23:1Z:25:LYS:O	2.16	0.45
28:15:52:ARG:HG3	28:15:54:VAL:HG13	1.98	0.45
1:1A:742:A:H2'	1:1A:743:A:C8	2.51	0.45
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.51	0.45
7:1H:9:VAL:O	7:1H:49:THR:HA	2.16	0.45
12:1O:58:LEU:HD11	12:1O:86:LEU:HD22	1.97	0.45
17:1T:106:LYS:HE3	17:1T:109:ARG:NH2	2.30	0.45
22:1Y:2:ALA:HA	22:1Y:85:PHE:HE2	1.80	0.45
1:1A:335:C:H5''	22:1Y:82:ARG:HD3	1.99	0.45
1:1A:1569:A:O4'	3:1D:59:LYS:NZ	2.39	0.45
1:1A:2772:C:H5'	4:1E:173:GLN:NE2	2.31	0.45
3:1D:261:LYS:HA	3:1D:264:ASP:OD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:72:ILE:HG23	8:1I:142:VAL:HG23	1.97	0.45
8:1I:115:VAL:HA	8:1I:132:PHE:CD1	2.52	0.45
10:1K:21:SER:O	10:1K:26:PRO:HD2	2.17	0.45
10:1K:80:LEU:HD23	10:1K:109:ILE:HD13	1.98	0.45
35:1c:156:ARG:HH12	35:1c:161:GLU:HA	1.81	0.45
43:1k:35:THR:OG1	43:1k:41:ALA:N	2.47	0.45
1:1A:155:A:H2'	1:1A:156:A:C8	2.52	0.45
1:1A:1832:C:C5'	33:1a:900:A:H4'	2.47	0.45
4:1E:25:THR:HG21	4:1E:193:VAL:HG22	1.97	0.45
6:1G:16:LEU:HD13	6:1G:29:PRO:HD2	1.98	0.45
8:1I:53:GLU:O	8:1I:57:LYS:HG2	2.16	0.45
41:1i:116:VAL:HG21	42:1j:62:ARG:HB2	1.99	0.45
45:1m:66:GLU:HG3	45:1m:67:GLY:H	1.80	0.45
1:1A:953:G:OP2	14:1Q:18[B]:ARG:NH1	2.50	0.45
1:1A:1224:U:H4'	19:1V:88:GLY:O	2.16	0.45
1:1A:2223:G:OP1	3:1D:171:TYR:OH	2.23	0.45
1:1A:2636:C:H4'	4:1E:81:GLU:OE1	2.17	0.45
1:1A:2667:C:H1'	7:1H:109:PHE:CD1	2.51	0.45
5:1F:151:GLY:HA3	5:1F:191:ASP:OD2	2.16	0.45
6:1G:73:SER:HB2	55:1x:67:C:H5'	1.98	0.45
21:1X:68:LYS:HZ1	21:1X:77:ARG:CZ	2.30	0.45
33:1a:875:U:C2'	40:1h:15:ARG:HH12	2.29	0.45
35:1c:172:ARG:HG2	35:1c:174:PRO:HD3	1.99	0.45
42:1j:49:PHE:HB2	42:1j:65:TYR:HB2	1.98	0.45
4:1E:99:GLU:HG2	4:1E:182:ALA:HB2	1.99	0.45
17:1T:43:PHE:HE2	17:1T:61:VAL:HB	1.80	0.45
29:16:25:LYS:NZ	29:16:51:GLU:OE1	2.38	0.45
30:17:34:ARG:HD3	30:17:42:LEU:HA	1.98	0.45
31:18:28:ASN:O	31:18:36:LYS:NZ	2.47	0.45
33:1a:154:U:O4	33:1a:155:A:N6	2.50	0.45
43:1k:16:VAL:HG12	43:1k:77:TYR:HB3	1.97	0.45
48:1p:16:PHE:HE2	48:1p:18:GLN:HE21	1.65	0.45
1:1A:79:C:O2'	1:1A:346:A:N3	2.44	0.45
1:1A:845:A:H5'	1:1A:846:U:OP2	2.17	0.45
1:1A:1442:U:H2'	1:1A:1443:U:C6	2.52	0.45
1:1A:2895:G:H2'	1:1A:2896:C:C6	2.52	0.45
2:1B:90:C:H5'	14:1Q:18[B]:ARG:CG	2.46	0.45
8:1I:127:GLU:HG2	8:1I:145:ASN:ND2	2.32	0.45
15:1R:10:LEU:HB3	15:1R:12:ARG:NH2	2.32	0.45
17:1T:22:PRO:HD3	17:1T:50:ILE:HD12	1.99	0.45
21:1X:6:ARG:O	21:1X:10:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1a:1347:G:N7	41:1i:12:ARG:NH2	2.53	0.45
40:1h:77:ARG:NH1	40:1h:126:ILE:HG23	2.31	0.45
49:1q:31:HIS:CD2	49:1q:34:TYR:H	2.32	0.45
1:1A:715:A:H1'	47:1o:60:VAL:HG11	1.98	0.45
14:1Q:56:ALA:HB2	14:1Q:119:LEU:HD12	1.99	0.45
21:1X:51:PHE:HZ	26:12:30:MET:HE2	1.82	0.45
33:1a:544:G:OP2	36:1d:63:ARG:NH2	2.50	0.45
33:1a:920:U:H2'	33:1a:921:U:C6	2.52	0.45
33:1a:1190:G:H5''	35:1c:176:HIS:HE1	1.82	0.45
53:1u:10:GLU:H	53:1u:11:PRO:CD	2.30	0.45
1:1A:1297:C:OP1	1:1A:2710:C:H4'	2.16	0.45
3:1D:43:ARG:HA	3:1D:48:ARG:O	2.17	0.45
3:1D:69:ARG:NH2	3:1D:116:ILE:HD12	2.32	0.45
9:1J:27:VAL:HG13	9:1J:80:THR:HG23	1.99	0.45
10:1K:53:LEU:HD21	10:1K:82:LYS:NZ	2.32	0.45
10:1K:119:GLY:O	10:1K:125:MET:HE3	2.17	0.45
11:1N:30:THR:O	11:1N:34:ARG:HG3	2.15	0.45
24:10:15:ASP:OD1	24:10:16:SER:N	2.49	0.45
33:1a:1052:U:O2'	33:1a:1055:A:OP2	2.29	0.45
33:1a:1237:C:H42	33:1a:1337:G:H1	1.64	0.45
39:1g:25:LYS:O	39:1g:29:ILE:HG12	2.17	0.45
45:1m:17:ILE:O	45:1m:20:THR:OG1	2.28	0.45
1:1A:26:G:C6	1:1A:27:G:N1	2.85	0.45
1:1A:464:U:H5'	30:17:5:PHE:CD1	2.52	0.45
1:1A:1794:A:H2'	1:1A:1795:C:C6	2.52	0.45
35:1c:151:VAL:HG12	35:1c:200:VAL:HG23	1.99	0.45
45:1m:4:ILE:O	45:1m:6:GLY:N	2.50	0.45
48:1p:6:LEU:HA	48:1p:19:VAL:HA	1.97	0.45
1:1A:1084:A:C8	9:1J:54:VAL:HB	2.52	0.44
1:1A:1418:G:H2'	1:1A:1579:A:N6	2.32	0.44
3:1D:34:LEU:HD21	3:1D:63:ARG:HD3	1.99	0.44
33:1a:427:U:OP1	36:1d:13:ARG:NH2	2.50	0.44
33:1a:754:C:OP1	47:1o:72:ARG:NH2	2.50	0.44
33:1a:1171:A:H2'	33:1a:1172:C:C6	2.52	0.44
33:1a:1356:G:H2'	33:1a:1357:A:C8	2.52	0.44
37:1e:137:VAL:O	37:1e:138:ARG:HB2	2.17	0.44
43:1k:87:LYS:HG2	43:1k:113:VAL:HG23	1.99	0.44
43:1k:126:LYS:O	43:1k:127:ARG:HB2	2.17	0.44
1:1A:523:C:H4'	1:1A:540:C:O2	2.17	0.44
2:1B:48:U:H2'	2:1B:49:C:C6	2.52	0.44
4:1E:4:LEU:HD22	4:1E:32:ASN:ND2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:49:ARG:NH1	5:1F:72:SER:HB3	2.32	0.44
5:1F:149:ILE:HB	5:1F:188:MET:HG2	1.99	0.44
8:1I:4:ILE:HG21	8:1I:47:PHE:CD2	2.51	0.44
33:1a:375:U:OP1	48:1p:70:ARG:NH1	2.40	0.44
33:1a:1256:A:H5''	35:1c:27:LYS:NZ	2.32	0.44
33:1a:1401:G:O6	33:1a:1504:G:N2	2.50	0.44
40:1h:95:VAL:HG12	40:1h:96:MET:HG3	1.99	0.44
41:1i:92:GLU:HB3	41:1i:95:ARG:NH1	2.32	0.44
46:1n:9:ARG:HG2	46:1n:13:ARG:NH1	2.32	0.44
47:1o:45:GLU:O	47:1o:47:LYS:N	2.50	0.44
1:1A:57:C:H2'	1:1A:58:G:O4'	2.17	0.44
1:1A:102:U:H2'	1:1A:102:U:O2	2.18	0.44
1:1A:518:G:O5'	20:1W:18:ARG:NH1	2.51	0.44
1:1A:572:A:H5'	19:1V:79:ARG:HH22	1.82	0.44
1:1A:1239:G:H2'	1:1A:1240:U:O4'	2.17	0.44
1:1A:1540:G:H2'	1:1A:1541:C:C6	2.53	0.44
1:1A:2772:C:H5'	4:1E:173:GLN:HE21	1.82	0.44
3:1D:171:TYR:HE1	3:1D:185:GLU:HB3	1.82	0.44
3:1D:201:MET:HG3	3:1D:202:LEU:HD12	1.98	0.44
5:1F:62:GLN:NE2	5:1F:69:ARG:HD2	2.30	0.44
6:1G:56:ASP:OD2	6:1G:150:ARG:NH2	2.51	0.44
17:1T:106:LYS:CE	17:1T:109:ARG:HH22	2.29	0.44
37:1e:24:THR:HA	37:1e:29:ARG:HA	1.99	0.44
1:1A:184:C:H2'	1:1A:185:G:C8	2.53	0.44
1:1A:1808:A:C5	25:11:28:ARG:NH1	2.86	0.44
1:1A:1869:G:H5'	1:1A:1870:C:OP2	2.18	0.44
3:1D:133:ARG:NH2	3:1D:187:ASP:OD1	2.51	0.44
15:1R:98:LEU:HD12	28:15:55:ILE:HD11	1.99	0.44
16:1S:17:LYS:O	16:1S:20:GLU:HG2	2.16	0.44
21:1X:70:HIS:N	21:1X:73:ARG:O	2.50	0.44
33:1a:575:G:O2'	33:1a:821:G:OP2	2.23	0.44
33:1a:946:A:H2'	33:1a:947:G:C8	2.53	0.44
35:1c:20:SER:HA	35:1c:57:ILE:O	2.17	0.44
35:1c:24:ALA:HB3	35:1c:29:PHE:HD1	1.83	0.44
37:1e:83:HIS:NE2	37:1e:147:MET:HG3	2.33	0.44
37:1e:150:PRO:HA	37:1e:153:VAL:HG22	1.99	0.44
47:1o:46:HIS:C	47:1o:48:LYS:H	2.24	0.44
1:1A:612:G:H2'	1:1A:614:A:C8	2.52	0.44
1:1A:1225:G:H4'	19:1V:86:GLN:HE21	1.81	0.44
1:1A:1847:G:H8	1:1A:1847:G:P	2.41	0.44
7:1H:69:ARG:NH1	7:1H:73:ASN:HB2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1J:103:ASN:C	9:1J:105:LYS:H	2.25	0.44
16:1S:71:ALA:HB2	16:1S:102:ARG:CG	2.46	0.44
18:1U:19:LYS:HG3	18:1U:22:LYS:HE2	2.00	0.44
33:1a:571:U:H5'	33:1a:819:A:C5	2.52	0.44
33:1a:1108:G:H5''	35:1c:176:HIS:CD2	2.52	0.44
33:1a:1366:C:O2'	42:1j:62:ARG:NH1	2.41	0.44
40:1h:9:ASP:O	40:1h:13:ARG:HG2	2.18	0.44
1:1A:1378:A:O2'	1:1A:1380:G:N7	2.46	0.44
3:1D:244:PRO:O	3:1D:252:THR:HG22	2.17	0.44
5:1F:59:PRO:HB2	5:1F:60:TRP:CE3	2.52	0.44
5:1F:168:ASP:OD2	5:1F:170:ARG:NH1	2.50	0.44
30:17:12:ARG:NH2	30:17:13:ASN:OD1	2.50	0.44
33:1a:236:A:H5''	49:1q:44:LEU:HD21	1.99	0.44
33:1a:662:U:O2'	33:1a:836:G:OP1	2.28	0.44
1:1A:851:C:OP1	27:13:19:LYS:HD3	2.18	0.44
6:1G:115:ARG:NH1	45:1m:68:ASP:OD1	2.50	0.44
27:13:40:ASP:OD1	27:13:45:ARG:NE	2.49	0.44
33:1a:1369:C:H2'	33:1a:1370:G:C8	2.53	0.44
34:1b:67:ILE:HD12	34:1b:160:ALA:HB3	1.99	0.44
37:1e:17:ALA:HB3	37:1e:36:LEU:HB3	1.99	0.44
37:1e:66:LYS:HA	37:1e:69:ARG:HH11	1.82	0.44
37:1e:157:ARG:O	37:1e:159:LYS:N	2.51	0.44
1:1A:301:G:P	22:1Y:82:ARG:HH12	2.41	0.44
1:1A:2031:A:C6	1:1A:2498:OMC:H1'	2.53	0.44
3:1D:171:TYR:CE1	3:1D:185:GLU:HB3	2.52	0.44
9:1J:32:GLY:O	9:1J:105:LYS:HD2	2.18	0.44
11:1N:142:ILE:HD12	11:1N:142:ILE:HA	1.74	0.44
23:1Z:51:GLN:NE2	23:1Z:86:LEU:HD21	2.29	0.44
33:1a:1342:C:H2'	33:1a:1343:G:C8	2.52	0.44
39:1g:66:LEU:O	39:1g:70:ARG:HG3	2.17	0.44
1:1A:550:C:C2'	1:1A:551:G:H5''	2.46	0.44
1:1A:1125:G:C6	1:1A:1126:A:N6	2.86	0.44
2:1B:28:C:OP1	16:1S:31:THR:HG21	2.18	0.44
9:1J:92:ALA:O	9:1J:95:LEU:N	2.51	0.44
10:1K:100:LYS:HA	10:1K:139:VAL:O	2.17	0.44
29:16:13:SER:HA	29:16:49:TYR:HD1	1.78	0.44
33:1a:1071:C:N4	33:1a:1104:G:H1	2.13	0.44
42:1j:78:GLU:HG3	42:1j:80:THR:H	1.83	0.44
42:1j:81:GLU:HA	42:1j:84:VAL:HG12	2.00	0.44
1:1A:725:G:C6	1:1A:726:G:N1	2.86	0.43
1:1A:2667:C:H1'	7:1H:109:PHE:HD1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:124:PHE:HE2	5:1F:157:LEU:HD11	1.81	0.43
8:1I:26:ALA:HA	8:1I:30:LEU:HB2	2.00	0.43
18:1U:21:ALA:HA	18:1U:24:TYR:CE2	2.53	0.43
18:1U:41:LYS:NZ	18:1U:45:TYR:OH	2.46	0.43
32:19:2:LYS:HB3	32:19:35:GLN:HG2	1.99	0.43
33:1a:677:U:O2	33:1a:777:A:O2'	2.32	0.43
33:1a:1505:G:H5'	33:1a:1506:U:H3'	2.00	0.43
33:1a:1526:G:OP2	53:1u:39:GLU:HB3	2.18	0.43
39:1g:65:ALA:HB1	39:1g:127:ALA:HB3	2.00	0.43
42:1j:9:ARG:NH1	42:1j:11:LYS:HD2	2.33	0.43
46:1n:20:TYR:CE2	46:1n:52:PRO:HG2	2.53	0.43
1:1A:1638:C:H4'	1:1A:2710:C:O2	2.17	0.43
1:1A:1750:G:O2'	1:1A:2860:A:N1	2.45	0.43
1:1A:2339:C:H2'	1:1A:2340:A:C8	2.53	0.43
3:1D:262:ARG:HG3	3:1D:263:THR:HG23	1.99	0.43
9:1J:113:PHE:CD2	9:1J:114:GLU:HG3	2.53	0.43
23:1Z:4:ILE:HG12	23:1Z:50:MET:HE1	2.00	0.43
33:1a:19:A:H2'	33:1a:20:U:C6	2.53	0.43
33:1a:451:A:H61	33:1a:481:G:H5'	1.83	0.43
33:1a:689:C:OP1	43:1k:29:ASN:ND2	2.51	0.43
33:1a:1147:C:H2'	33:1a:1148:U:C6	2.54	0.43
42:1j:40:ILE:HD12	42:1j:73:LEU:HD22	2.01	0.43
49:1q:46:VAL:HG13	49:1q:74:THR:HA	2.00	0.43
51:1s:28:LYS:HG3	51:1s:29:LYS:H	1.83	0.43
53:1u:4:ILE:HD13	53:1u:19:PHE:HE2	1.82	0.43
1:1A:58:G:O2'	1:1A:73:A:N1	2.45	0.43
1:1A:493:G:H2'	1:1A:494:G:O4'	2.18	0.43
1:1A:1881:C:H2'	1:1A:1882:U:O4'	2.18	0.43
1:1A:2017:U:H4'	28:15:5:GLN:O	2.18	0.43
1:1A:2636:C:H2'	1:1A:2637:U:C6	2.53	0.43
4:1E:118:PHE:CE1	4:1E:163:GLY:HA2	2.53	0.43
4:1E:186:LEU:HD23	4:1E:186:LEU:HA	1.81	0.43
11:1N:31:GLU:CD	11:1N:34:ARG:HH11	2.25	0.43
24:10:72:LYS:HB2	24:10:79:PHE:CE2	2.53	0.43
25:11:4:VAL:HG22	25:11:11:ARG:HE	1.83	0.43
52:1t:35:VAL:HG21	52:1t:54:MET:SD	2.58	0.43
55:1x:54:G:H2'	55:1x:55:G:C8	2.54	0.43
1:1A:1223:G:N1	1:1A:1226:A:OP2	2.49	0.43
1:1A:2039:U:H2'	1:1A:2040:G:C8	2.54	0.43
4:1E:56:LYS:HB3	4:1E:56:LYS:HE3	1.79	0.43
5:1F:70:SER:HB2	5:1F:78:TRP:CZ2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1T:43:PHE:CE1	17:1T:63:LYS:HE3	2.53	0.43
42:1j:27:GLU:HA	42:1j:30:LYS:HE3	1.99	0.43
42:1j:51:VAL:HB	46:1n:81:ARG:HB2	1.99	0.43
45:1m:54:ASP:OD1	45:1m:55:THR:N	2.51	0.43
1:1A:372:G:O2'	25:11:54:LYS:NZ	2.39	0.43
1:1A:518:G:H4'	20:1W:18:ARG:CZ	2.49	0.43
19:1V:68:ARG:HH11	19:1V:90:ARG:HB2	1.83	0.43
33:1a:427:U:O2'	33:1a:541:G:OP1	2.36	0.43
33:1a:603:U:H2'	33:1a:604:G:C8	2.53	0.43
35:1c:19:ASN:OD1	35:1c:54:ARG:NH2	2.51	0.43
36:1d:14:ARG:HG3	36:1d:56:ARG:NH1	2.33	0.43
39:1g:105:VAL:O	39:1g:109:ARG:HG2	2.19	0.43
41:1i:60:LYS:NZ	41:1i:61:LEU:HD23	2.33	0.43
43:1k:53:ARG:HH11	43:1k:57:LYS:HE2	1.82	0.43
49:1q:59:VAL:HG23	49:1q:78:VAL:HG22	2.00	0.43
1:1A:575:A:OP2	1:1A:2499:C:O2'	2.36	0.43
1:1A:651:G:H5'	31:18:19:LYS:HG3	2.01	0.43
1:1A:720:U:H2'	1:1A:721:A:C8	2.53	0.43
1:1A:1447:C:H2'	1:1A:1448:G:C8	2.53	0.43
1:1A:2532:G:O2'	1:1A:2657:A:N1	2.50	0.43
1:1A:2886[A]:A:C6	1:1A:2887[A]:A:C5	3.07	0.43
6:1G:105:THR:HG22	6:1G:106:ILE:HG23	1.99	0.43
6:1G:113:ASP:OD1	45:1m:66:GLU:HG3	2.19	0.43
15:1R:102:PHE:HD1	15:1R:109:PRO:HA	1.84	0.43
33:1a:539:A:H2'	33:1a:540:G:C8	2.53	0.43
33:1a:1201:A:H4'	33:1a:1202:U:O5'	2.18	0.43
33:1a:1488:G:H2'	33:1a:1489:G:H8	1.83	0.43
34:1b:138:THR:HA	34:1b:141:LEU:HD13	2.00	0.43
45:1m:8:ASN:ND2	45:1m:21:SER:HB3	2.33	0.43
1:1A:1007:C:H5''	11:1N:37:ARG:HH21	1.84	0.43
1:1A:2800:A:C2	1:1A:2895:G:H1'	2.54	0.43
3:1D:175:ARG:HH22	33:1a:713:G:H5'	1.83	0.43
5:1F:90:GLN:HG3	5:1F:92:HIS:CE1	2.54	0.43
13:1P:123:ARG:NH2	13:1P:143:GLU:OE2	2.49	0.43
36:1d:124:MET:HG3	36:1d:146:ARG:HG2	2.00	0.43
36:1d:124:MET:HA	36:1d:129:VAL:HA	1.99	0.43
52:1t:60:ARG:O	52:1t:64:LYS:HG2	2.19	0.43
53:1u:4:ILE:HG23	53:1u:20:LYS:HE3	2.00	0.43
1:1A:1997:C:OP2	4:1E:129:THR:OG1	2.29	0.43
1:1A:2591:C:H2'	1:1A:2592:G:C8	2.54	0.43
3:1D:210:ALA:O	3:1D:214:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1J:68:PRO:HD2	9:1J:69:PHE:CE2	2.53	0.43
27:13:41:THR:OG1	27:13:44:ILE:HG12	2.18	0.43
1:1A:1187:G:H5''	19:1V:83:TYR:CZ	2.54	0.43
1:1A:2386:A:C2	24:10:41[A]:ARG:HG3	2.53	0.43
1:1A:2394:C:H5''	13:1P:63:LYS:HE2	2.00	0.43
3:1D:144:VAL:HB	3:1D:154:LEU:HB2	2.00	0.43
11:1N:72:LYS:HE3	11:1N:74:TYR:HE1	1.84	0.43
24:10:37:ILE:HG21	24:10:80:ILE:HG21	2.01	0.43
31:18:39:LYS:HG3	31:18:42:ARG:NH1	2.34	0.43
33:1a:766:A:OP2	33:1a:812:G:N2	2.51	0.43
33:1a:1271:A:H2'	33:1a:1272:G:C8	2.53	0.43
51:1s:3:ARG:NH2	51:1s:68:GLY:O	2.52	0.43
1:1A:191:A:H2'	1:1A:192:C:C6	2.54	0.43
1:1A:545:U:H3'	1:1A:546:U:H4'	2.01	0.43
1:1A:728:G:H4'	3:1D:13:ARG:CD	2.46	0.43
1:1A:1095:A:H61	10:1K:30:GLN:NE2	2.13	0.43
6:1G:36:LEU:HD12	6:1G:61:SER:HB3	2.00	0.43
23:1Z:47:VAL:O	23:1Z:51:GLN:HG2	2.19	0.43
33:1a:933:G:OP2	39:1g:3:ARG:HB3	2.18	0.43
38:1f:47:LEU:HD13	38:1f:51:ILE:HG12	2.00	0.43
39:1g:15:ASP:OD1	39:1g:44:TYR:OH	2.37	0.43
1:1A:1182:G:H2'	1:1A:1183:U:O4'	2.19	0.42
1:1A:1746:A:H2'	1:1A:1747:U:C6	2.54	0.42
1:1A:2262:U:OP2	24:10:19:LYS:NZ	2.50	0.42
6:1G:67:ILE:O	6:1G:67:ILE:HG13	2.19	0.42
6:1G:73:SER:CB	6:1G:80:ARG:HA	2.48	0.42
8:1I:142:VAL:HG12	8:1I:143:ILE:N	2.34	0.42
13:1P:132:ARG:HG3	13:1P:142:ILE:HD13	2.00	0.42
18:1U:44:GLN:NE2	19:1V:77:PHE:HD2	2.17	0.42
20:1W:39:THR:HG22	20:1W:41:LYS:HG2	2.00	0.42
28:15:34:SER:HB3	28:15:48:TYR:CD2	2.54	0.42
31:18:42:ARG:HA	31:18:45:ARG:NH1	2.34	0.42
33:1a:413:G:H1'	33:1a:428:G:N2	2.34	0.42
33:1a:1211:U:H4'	33:1a:1212:U:O5'	2.18	0.42
33:1a:1253:G:N2	33:1a:1355:G:O3'	2.44	0.42
34:1b:82:ASP:N	34:1b:82:ASP:OD1	2.52	0.42
37:1e:82:GLN:OE1	37:1e:149:SER:HA	2.19	0.42
42:1j:11:LYS:HG2	42:1j:71:LEU:HG	2.01	0.42
50:1r:38:LYS:HD2	53:1u:24:GLU:OE2	2.19	0.42
1:1A:335:C:OP2	22:1Y:82:ARG:NH2	2.53	0.42
1:1A:362:A:H3'	1:1A:363:G:H8	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1417:C:H2'	1:1A:1418:G:O4'	2.19	0.42
1:1A:1992:G:N2	1:1A:1996:C:O2'	2.52	0.42
1:1A:2600:A:N7	3:1D:236:GLU:HG2	2.34	0.42
1:1A:2819:G:H2'	1:1A:2821:A:N7	2.34	0.42
4:1E:13:ARG:HG2	17:1T:56:HIS:CE1	2.53	0.42
5:1F:73:ILE:HA	5:1F:78:TRP:HZ3	1.81	0.42
6:1G:40:VAL:HG23	6:1G:86:GLY:HA2	2.01	0.42
33:1a:332:G:OP2	52:1t:3:ASN:HB3	2.19	0.42
33:1a:513:C:H2'	33:1a:514:C:C6	2.54	0.42
33:1a:837:U:H2'	33:1a:838:G:H8	1.84	0.42
33:1a:855:U:OP2	33:1a:871:U:N3	2.35	0.42
41:1i:52:LEU:HD13	41:1i:57:MET:SD	2.60	0.42
46:1n:16:LEU:HD22	46:1n:20:TYR:CE2	2.54	0.42
1:1A:2184:A:H2'	1:1A:2185:U:C6	2.53	0.42
7:1H:95:ARG:HD2	7:1H:128:GLN:CB	2.46	0.42
14:1Q:51:ARG:O	14:1Q:55:ARG:NH1	2.52	0.42
23:1Z:51:GLN:CD	23:1Z:86:LEU:HD11	2.44	0.42
26:12:26:PHE:HD1	26:12:29:ARG:NH1	2.15	0.42
33:1a:309:A:H2'	33:1a:310:G:H8	1.83	0.42
33:1a:505:G:OP2	33:1a:535:A:H5'	2.19	0.42
33:1a:1123:U:O2'	42:1j:39:PRO:O	2.34	0.42
33:1a:1314:C:OP2	51:1s:6:LYS:HD3	2.19	0.42
38:1f:42:TRP:HB2	38:1f:59:TYR:HB2	2.01	0.42
1:1A:833:A:H2'	1:1A:834:G:C8	2.54	0.42
12:1O:71:ARG:HH22	12:1O:123:LEU:C	2.27	0.42
33:1a:1512:U:H2'	33:1a:1513:A:C8	2.53	0.42
39:1g:66:LEU:HD23	39:1g:70:ARG:HE	1.84	0.42
40:1h:29:SER:HB3	40:1h:57:PRO:HB2	2.00	0.42
40:1h:75:ILE:HD12	40:1h:128:TYR:O	2.18	0.42
42:1j:50:THR:HA	42:1j:64:GLN:HA	2.01	0.42
1:1A:280:U:H2'	1:1A:281:C:C6	2.54	0.42
1:1A:1799:G:H3'	3:1D:258:ARG:HH12	1.84	0.42
1:1A:1806:C:H1'	3:1D:44:ASN:HD21	1.83	0.42
1:1A:2117:A:H61	1:1A:2171:A:H61	1.66	0.42
10:1K:93:PRO:HB3	10:1K:137:GLY:N	2.34	0.42
13:1P:78:ARG:HG2	13:1P:113:ALA:HB3	2.02	0.42
25:11:18:ARG:NH2	25:11:24:ALA:HB2	2.31	0.42
28:15:48:TYR:CE1	28:15:53:LYS:HD3	2.54	0.42
33:1a:709:U:H2'	33:1a:710:G:H8	1.84	0.42
33:1a:950:U:H2'	33:1a:951:G:H8	1.82	0.42
52:1t:39:ILE:HG21	52:1t:82:GLN:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1365:A:OP1	25:11:28:ARG:NH2	2.46	0.42
1:1A:2020:A:H5'	28:15:9:THR:HG22	2.02	0.42
1:1A:2849:U:H4'	1:1A:2868:A:C2	2.55	0.42
4:1E:13:ARG:NH1	17:1T:56:HIS:HA	2.34	0.42
9:1J:103:ASN:O	9:1J:105:LYS:N	2.52	0.42
21:1X:6:ARG:HH22	21:1X:37:ASP:CG	2.27	0.42
21:1X:34:VAL:HG21	21:1X:43:ILE:HD11	2.01	0.42
33:1a:692:U:H2'	33:1a:694:A:OP2	2.19	0.42
33:1a:1064:G:N2	33:1a:1190:G:H1'	2.35	0.42
33:1a:1437:A:H2'	33:1a:1438:G:C8	2.55	0.42
36:1d:162:ALA:O	36:1d:167:LYS:HE3	2.20	0.42
53:1u:40:LYS:HB3	53:1u:41:PRO:HD3	2.02	0.42
1:1A:1665:A:O2'	12:1O:1:MET:HB3	2.19	0.42
1:1A:1796:U:H2'	1:1A:1797:G:H8	1.84	0.42
1:1A:2566:A:H4'	1:1A:2567:G:H5''	2.01	0.42
3:1D:161:TYR:HB3	3:1D:194:GLU:HG2	2.02	0.42
7:1H:94:TYR:CD1	7:1H:107:LEU:HA	2.55	0.42
8:1I:85:GLY:HA2	8:1I:91:PHE:CZ	2.55	0.42
12:1O:2:ILE:HD12	12:1O:8:LEU:HD11	2.02	0.42
13:1P:85:VAL:HB	13:1P:94:THR:CG2	2.48	0.42
16:1S:53:THR:HB	16:1S:65:THR:HB	2.02	0.42
33:1a:1201:A:H1'	33:1a:1202:U:OP2	2.19	0.42
36:1d:201:VAL:HG11	37:1e:103:THR:HB	2.02	0.42
1:1A:139:U:O2'	1:1A:141:G:N1	2.51	0.42
1:1A:1650:A:H4'	15:1R:103:ARG:NH2	2.34	0.42
1:1A:2831:G:OP1	4:1E:56:LYS:HE2	2.20	0.42
6:1G:75:ALA:HA	55:1x:67:C:O2'	2.19	0.42
17:1T:71:GLU:OE2	17:1T:101:ARG:NE	2.52	0.42
33:1a:826:C:O2	40:1h:16:ASN:ND2	2.53	0.42
33:1a:932:C:OP1	39:1g:4:ARG:HB2	2.20	0.42
33:1a:1279:G:OP1	42:1j:9:ARG:NH2	2.52	0.42
33:1a:1502:A:N6	33:1a:1505:G:H1	2.17	0.42
33:1a:1503:A:H5'	33:1a:1531:A:H1'	2.02	0.42
36:1d:58:LYS:HD3	36:1d:203:LEU:HD23	2.01	0.42
48:1p:70:ARG:O	48:1p:74:LEU:HG	2.20	0.42
1:1A:394:C:N4	1:1A:395:U:O4	2.53	0.42
1:1A:927:A:O2'	27:13:39:GLU:OE2	2.35	0.42
1:1A:933:A:H5'	1:1A:934:U:OP2	2.20	0.42
9:1J:107:GLU:O	9:1J:108:VAL:HB	2.19	0.42
10:1K:117:MET:HB2	10:1K:125:MET:HE2	2.02	0.42
13:1P:85:VAL:HG21	13:1P:90:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1R:35:LYS:HE3	15:1R:100:CYS:SG	2.59	0.42
33:1a:458:U:H2'	33:1a:459:A:C8	2.55	0.42
35:1c:150:LYS:HB3	35:1c:201:TRP:HB2	2.02	0.42
37:1e:12:GLN:HG3	37:1e:117:VAL:HG12	2.02	0.42
37:1e:12:GLN:HB3	37:1e:40:GLY:O	2.20	0.42
38:1f:5:GLU:HG3	38:1f:63:ASN:HD21	1.85	0.42
1:1A:12:U:O2	1:1A:12:U:H2'	2.20	0.42
1:1A:372:G:H5''	25:11:61:LYS:HD3	2.01	0.42
3:1D:79:GLU:OE2	3:1D:95:LEU:HB2	2.20	0.42
4:1E:149:ASN:CG	4:1E:150[A]:MEQ:H	2.27	0.42
13:1P:56:PRO:O	13:1P:60:ARG:HG3	2.20	0.42
26:12:25:GLN:O	26:12:29:ARG:HG3	2.20	0.42
33:1a:151:A:OP2	33:1a:169:C:N4	2.34	0.42
33:1a:229:U:H2'	33:1a:230:G:C8	2.55	0.42
33:1a:413:G:N2	33:1a:428:G:H1'	2.34	0.42
34:1b:31:ILE:HG23	34:1b:39:HIS:HB3	2.01	0.42
34:1b:73:LYS:O	34:1b:77:SER:OG	2.36	0.42
48:1p:71:VAL:O	48:1p:75:ILE:HD12	2.20	0.42
1:1A:937:C:OP1	31:18:52:LYS:HD2	2.20	0.41
3:1D:71:LYS:HZ1	3:1D:98:ASP:CG	2.25	0.41
3:1D:201:MET:HE3	3:1D:201:MET:HB2	1.79	0.41
9:1J:65:GLU:HA	9:1J:70:GLU:HG2	2.01	0.41
11:1N:47:HIS:CE1	11:1N:48:VAL:HG23	2.55	0.41
27:13:45:ARG:HH22	27:13:57:VAL:HG11	1.85	0.41
33:1a:22:G:H4'	33:1a:885:G:C8	2.55	0.41
33:1a:1488:G:H2'	33:1a:1489:G:C8	2.55	0.41
1:1A:118:A:N3	1:1A:178:G:H1'	2.35	0.41
1:1A:1385:A:O2'	1:1A:1396:U:O2	2.36	0.41
1:1A:1932:A:H2'	1:1A:1933:G:O4'	2.20	0.41
1:1A:2095:A:H2'	1:1A:2096:C:O4'	2.20	0.41
1:1A:2346:A:H3'	1:1A:2347:C:H5''	2.01	0.41
3:1D:29:PRO:HG2	3:1D:34:LEU:HD11	2.03	0.41
9:1J:8:LYS:HB2	9:1J:8:LYS:HE2	1.87	0.41
9:1J:31:ARG:NE	9:1J:79:PRO:HG3	2.31	0.41
27:13:5:ILE:HG21	27:13:45:ARG:NH1	2.35	0.41
27:13:17:LEU:HD12	27:13:20:HIS:CE1	2.55	0.41
33:1a:1391:U:H2'	33:1a:1392:G:C8	2.55	0.41
33:1a:1436:U:O4	33:1a:1437:A:N6	2.53	0.41
33:1a:1467:C:H2'	33:1a:1468:A:H8	1.85	0.41
51:1s:52:HIS:HD2	51:1s:57:HIS:CE1	2.38	0.41
1:1A:388:G:N7	1:1A:390:U:H2'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2054:A:H2'	28:15:5:GLN:OE1	2.20	0.41
1:1A:2530:A:N6	7:1H:156:PRO:HG3	2.35	0.41
2:1B:104:A:H2'	2:1B:105:G:O4'	2.20	0.41
5:1F:26:ALA:HB2	13:1P:9:ALA:HB2	2.02	0.41
11:1N:31:GLU:OE2	11:1N:35:ARG:NE	2.53	0.41
22:1Y:89:ASP:CG	22:1Y:90:GLY:H	2.27	0.41
31:18:7:VAL:HB	31:18:61:CYS:HB3	2.01	0.41
33:1a:199:A:H2'	33:1a:200:G:H8	1.85	0.41
33:1a:337:G:H2'	33:1a:338:A:C8	2.54	0.41
33:1a:736:C:O4'	38:1f:88:MET:HE2	2.20	0.41
37:1e:96:MET:HE1	37:1e:140:THR:HG23	2.02	0.41
49:1q:8:LEU:HD23	49:1q:25:ILE:HG21	2.02	0.41
1:1A:576:U:H2'	1:1A:577:G:C8	2.55	0.41
1:1A:2728:U:O2'	1:1A:2729:G:H5''	2.20	0.41
1:1A:2751:G:OP2	7:1H:3:ARG:HD2	2.19	0.41
2:1B:66:A:N6	2:1B:107:G:H2'	2.35	0.41
7:1H:52:PHE:HZ	7:1H:72:LEU:HD22	1.83	0.41
10:1K:106:LEU:HD11	10:1K:140:VAL:HG11	2.01	0.41
33:1a:458:U:H2'	33:1a:459:A:H8	1.85	0.41
33:1a:679:C:H42	33:1a:711:G:H1	1.67	0.41
33:1a:976:G:OP2	33:1a:1358:U:O2'	2.37	0.41
33:1a:1347:G:O2'	33:1a:1373:G:O6	2.38	0.41
39:1g:150:ALA:HB1	43:1k:59:THR:HG21	2.02	0.41
1:1A:2262:U:H5''	24:10:41[A]:ARG:HH12	1.84	0.41
1:1A:2311:A:C2	6:1G:77:PHE:HB3	2.56	0.41
1:1A:2489:U:C4	1:1A:2490:G:C6	3.09	0.41
7:1H:166:ASP:OD1	7:1H:167:GLU:N	2.54	0.41
7:1H:170:ARG:NH2	32:19:29:ALA:O	2.42	0.41
14:1Q:55:ARG:HH11	14:1Q:55:ARG:HB2	1.85	0.41
19:1V:41:ILE:HD13	19:1V:103:ALA:HA	2.02	0.41
31:18:62:LEU:HB3	31:18:65:ALA:HB2	2.02	0.41
33:1a:219:U:H2'	33:1a:220:G:C8	2.56	0.41
35:1c:58:GLU:OE2	35:1c:65:ARG:HD2	2.20	0.41
41:1i:18:ARG:HH21	41:1i:20:PHE:HZ	1.67	0.41
44:1l:114:ARG:HH22	44:1l:121:ARG:HH11	1.67	0.41
46:1n:9:ARG:HG2	46:1n:13:ARG:HH12	1.85	0.41
1:1A:588:U:H2'	1:1A:589:U:C6	2.55	0.41
1:1A:634:C:H2'	1:1A:635:C:C6	2.55	0.41
1:1A:1175:A:N3	1:1A:1175:A:H2'	2.36	0.41
1:1A:2328:A:H2'	1:1A:2329:U:C6	2.55	0.41
6:1G:113:ASP:CG	45:1m:66:GLU:HG3	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:16:17:THR:HG21	29:16:42:VAL:HB	2.02	0.41
33:1a:1163:A:H2'	33:1a:1164:G:C8	2.56	0.41
36:1d:60:LYS:O	36:1d:64:ILE:HG13	2.20	0.41
1:1A:45:G:N7	1:1A:215:G:O2'	2.49	0.41
1:1A:1539:U:H2'	1:1A:1540:G:C8	2.56	0.41
1:1A:1740:G:H2'	1:1A:1741:C:O4'	2.21	0.41
1:1A:2168:G:N3	1:1A:2168:G:H2'	2.34	0.41
1:1A:2272:U:H5''	1:1A:2273:A:OP1	2.21	0.41
1:1A:2576:G:O2'	1:1A:2579:C:OP2	2.32	0.41
4:1E:55:LYS:HD3	4:1E:60:VAL:HG22	2.03	0.41
5:1F:154:ASP:HB3	5:1F:157:LEU:HB3	2.01	0.41
10:1K:81:LYS:HG3	10:1K:136:MET:HE1	2.02	0.41
11:1N:118:MET:HA	11:1N:121:LYS:HZ1	1.84	0.41
17:1T:4:ILE:H	17:1T:4:ILE:HD12	1.85	0.41
30:17:34:ARG:HG3	30:17:39:ARG:CG	2.41	0.41
33:1a:309:A:H2'	33:1a:310:G:C8	2.56	0.41
33:1a:536:C:N4	33:1a:537:G:O6	2.53	0.41
33:1a:598:U:H4'	40:1h:86:TYR:CD2	2.56	0.41
33:1a:1087:G:N2	33:1a:1099:G:H1'	2.36	0.41
33:1a:1458:G:H5'	52:1t:27:MET:HB3	2.02	0.41
34:1b:20:THR:OG1	34:1b:37:LYS:O	2.30	0.41
36:1d:15:GLU:HG3	36:1d:19:LEU:HD11	2.01	0.41
43:1k:50:SER:HA	43:1k:69:ARG:NH1	2.35	0.41
1:1A:48:G:N2	1:1A:49:A:N1	2.68	0.41
1:1A:544:C:H3'	1:1A:545:U:C2	2.56	0.41
1:1A:747:5MU:O2	1:1A:2014:A:H1'	2.20	0.41
1:1A:1199:U:H2'	1:1A:1200:C:C6	2.54	0.41
1:1A:2324:U:H3'	1:1A:2325:G:H5''	2.02	0.41
1:1A:2822:G:O6	15:1R:2:ARG:HD3	2.20	0.41
2:1B:90:C:H5'	14:1Q:18[B]:ARG:HG2	2.01	0.41
4:1E:38:LYS:O	4:1E:46:ARG:HA	2.20	0.41
11:1N:136:GLN:H	11:1N:136:GLN:HG3	1.30	0.41
13:1P:19:LEU:HD23	13:1P:27:LEU:HB3	2.02	0.41
18:1U:44:GLN:HE22	19:1V:77:PHE:HD2	1.67	0.41
23:1Z:21:ARG:HE	23:1Z:87:GLN:HA	1.85	0.41
23:1Z:53:LYS:HB3	23:1Z:55:GLU:OE1	2.21	0.41
24:10:41[B]:ARG:HA	24:10:41[B]:ARG:HD3	1.88	0.41
31:18:16:LYS:HA	31:18:22:PHE:CD1	2.54	0.41
33:1a:652:U:O4	33:1a:752:G:O2'	2.30	0.41
37:1e:96:MET:HE2	37:1e:111:MET:HE3	2.02	0.41
50:1r:29:LEU:HD23	50:1r:59:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1s:44:MET:HA	51:1s:47:LEU:HD12	2.03	0.41
1:1A:30:G:OP2	18:1U:5:LYS:NZ	2.39	0.41
1:1A:608:A:C6	1:1A:609:A:C6	3.08	0.41
1:1A:640:C:H2'	1:1A:641:U:C6	2.56	0.41
1:1A:1585:C:H2'	1:1A:1586:A:O4'	2.21	0.41
1:1A:1655:A:H1'	4:1E:118:PHE:CD2	2.56	0.41
1:1A:1817:G:H5''	3:1D:87:ARG:CG	2.50	0.41
4:1E:47:ALA:HA	4:1E:84:LEU:HG	2.03	0.41
4:1E:52:THR:HG23	4:1E:77:ARG:NH2	2.36	0.41
7:1H:26:ILE:HG22	7:1H:79:VAL:HG21	2.03	0.41
10:1K:117:MET:HG3	10:1K:125:MET:HB3	2.02	0.41
15:1R:28:LEU:HD23	15:1R:48:VAL:HG11	2.03	0.41
19:1V:61:ALA:HB2	19:1V:98:ILE:HD13	2.03	0.41
23:1Z:74:ALA:HA	23:1Z:91:PHE:HD1	1.86	0.41
24:10:69:PHE:CD1	24:10:80:ILE:HG12	2.56	0.41
29:16:19:HIS:HE1	29:16:21:TYR:CE1	2.39	0.41
33:1a:925:G:H2'	33:1a:927:G:H8	1.86	0.41
34:1b:193:PRO:HB2	34:1b:194:ASP:H	1.66	0.41
37:1e:39:VAL:HG22	37:1e:67:ALA:HB1	2.03	0.41
41:1i:107:ASP:OD1	41:1i:109:ARG:NE	2.53	0.41
43:1k:23:ILE:HG22	43:1k:32:VAL:HG13	2.03	0.41
43:1k:85:MET:HA	43:1k:111:THR:O	2.21	0.41
43:1k:101:ASN:OD1	43:1k:102:ALA:N	2.54	0.41
44:1l:74:LEU:HD21	44:1l:80:ILE:HG21	2.03	0.41
47:1o:53:ARG:O	47:1o:57:LEU:HG	2.20	0.41
1:1A:629:G:H4'	1:1A:650:C:O2	2.21	0.41
1:1A:686:U:H2'	1:1A:788:A:N1	2.36	0.41
1:1A:1173:U:O2'	1:1A:1174:U:O5'	2.33	0.41
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.55	0.41
1:1A:1939:5MU:OP1	1:1A:2604:PSU:O2'	2.35	0.41
1:1A:2451:A:H4'	55:1x:87:A:C5	2.56	0.41
11:1N:32:LEU:O	11:1N:36:LEU:HG	2.20	0.41
28:15:9:THR:OG1	28:15:12:LYS:HG2	2.21	0.41
33:1a:211:G:H2'	33:1a:211:G:N3	2.36	0.41
39:1g:130:ASN:C	39:1g:135:VAL:HG21	2.45	0.41
41:1i:51:PRO:HB3	41:1i:84:THR:HG22	2.03	0.41
43:1k:50:SER:HA	43:1k:69:ARG:HH11	1.86	0.41
54:1v:17:U:H6	54:1v:17:U:O5'	2.04	0.41
1:1A:945:A:C4	1:1A:2448:A:C2	3.09	0.40
1:1A:1494:A:HO2'	1:1A:1495:A:P	2.43	0.40
1:1A:1796:U:H2'	1:1A:1797:G:C8	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1a:925:G:H1	33:1a:1391:U:H3	1.69	0.40
34:1b:96:TRP:CZ3	34:1b:98:GLY:HA2	2.56	0.40
35:1c:7:PRO:HD2	35:1c:184:TYR:CD2	2.56	0.40
41:1i:26:GLY:H	41:1i:59:GLU:CG	2.34	0.40
42:1j:9:ARG:HH12	42:1j:11:LYS:HD2	1.84	0.40
42:1j:40:ILE:HG22	42:1j:42:LEU:HG	2.03	0.40
47:1o:36:ILE:HD13	47:1o:60:VAL:HG22	2.03	0.40
1:1A:729:G:C5	3:1D:207:LYS:HB2	2.57	0.40
1:1A:851:C:H2'	1:1A:852:U:H6	1.86	0.40
1:1A:994:C:H3'	18:1U:54:LYS:HE3	2.03	0.40
1:1A:1913:A:N6	33:1a:1492:A:N3	2.64	0.40
1:1A:2069:G7M:C2'	1:1A:2070:A:O5'	2.69	0.40
5:1F:195:GLN:O	5:1F:199:MET:HG3	2.21	0.40
18:1U:36:PHE:HZ	19:1V:84:ARG:HH22	1.69	0.40
36:1d:187:GLU:HG3	36:1d:189:SER:H	1.85	0.40
40:1h:104:VAL:HA	40:1h:125:ILE:HA	2.02	0.40
43:1k:19:GLY:O	43:1k:82:LEU:HA	2.21	0.40
1:1A:2312:U:H2'	6:1G:37:ASN:HD21	1.86	0.40
1:1A:2528:U:H2'	1:1A:2530:A:O5'	2.22	0.40
9:1J:29:ASP:OD1	9:1J:79:PRO:HG2	2.20	0.40
10:1K:32:GLY:O	10:1K:65:ARG:HB3	2.22	0.40
28:15:36:GLU:OE1	28:15:44:THR:HB	2.21	0.40
33:1a:35:G:H2'	33:1a:36:C:C6	2.57	0.40
33:1a:1255:G:O2'	33:1a:1258:G:N3	2.45	0.40
47:1o:56:LEU:O	47:1o:60:VAL:HG23	2.21	0.40
1:1A:17:G:H2'	1:1A:18:U:C6	2.57	0.40
1:1A:620:G:H4'	1:1A:621:A:O5'	2.22	0.40
1:1A:1664:A:C2	12:1O:1:MET:HE1	2.53	0.40
1:1A:2356:U:O3'	24:10:20:ARG:HD3	2.22	0.40
3:1D:142:HIS:HD2	3:1D:193:GLY:C	2.29	0.40
14:1Q:52:ALA:O	14:1Q:56:ALA:N	2.54	0.40
16:1S:51:ALA:HB3	16:1S:78:VAL:HG13	2.04	0.40
22:1Y:87:PHE:CE1	22:1Y:92:LYS:HE2	2.54	0.40
23:1Z:14:LYS:HD3	23:1Z:18:ARG:NH2	2.36	0.40
33:1a:193:C:H2'	33:1a:194:C:C6	2.57	0.40
33:1a:468:A:H5'	33:1a:469:C:OP2	2.22	0.40
33:1a:591:U:H2'	33:1a:592:G:C8	2.56	0.40
33:1a:601:G:H2'	33:1a:602:A:H8	1.86	0.40
33:1a:916:U:H2'	33:1a:917:G:C8	2.56	0.40
1:1A:634:C:H6	1:1A:634:C:O5'	2.05	0.40
1:1A:910:A:C6	1:1A:911:A:C6	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:934:U:H2'	1:1A:935:C:C6	2.56	0.40
1:1A:1083:U:C4'	9:1J:42:ARG:HH12	2.22	0.40
1:1A:1367:A:O2'	30:17:25:LYS:HE3	2.22	0.40
1:1A:2305:U:O2'	6:1G:133:ARG:NE	2.55	0.40
2:1B:48:U:P	16:1S:30:ARG:NH2	2.93	0.40
3:1D:24:LEU:HD23	3:1D:83:TYR:HB2	2.03	0.40
8:1I:121:VAL:O	8:1I:121:VAL:HG12	2.22	0.40
9:1J:38:MET:O	9:1J:42:ARG:HG2	2.20	0.40
33:1a:216:U:H2'	33:1a:217:C:C6	2.57	0.40
33:1a:426:U:H2'	33:1a:427:U:C6	2.56	0.40
33:1a:916:U:H2'	33:1a:917:G:H8	1.86	0.40
34:1b:128:LYS:HE3	34:1b:129:LEU:HG	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	269/273 (98%)	251 (93%)	17 (6%)	1 (0%)	30	61
4	1E	206/209 (99%)	200 (97%)	6 (3%)	0	100	100
5	1F	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
6	1G	175/179 (98%)	164 (94%)	11 (6%)	0	100	100
7	1H	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
8	1I	147/149 (99%)	132 (90%)	13 (9%)	2 (1%)	9	38
9	1J	133/165 (81%)	114 (86%)	13 (10%)	6 (4%)	2	17
10	1K	132/142 (93%)	122 (92%)	6 (4%)	4 (3%)	3	25
11	1N	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
12	1O	121/123 (98%)	116 (96%)	4 (3%)	1 (1%)	16	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	1P	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
14	1Q	136/136 (100%)	126 (93%)	8 (6%)	2 (2%)	8	37
15	1R	123/127 (97%)	117 (95%)	5 (4%)	1 (1%)	16	49
16	1S	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
17	1T	112/115 (97%)	108 (96%)	3 (3%)	1 (1%)	14	46
18	1U	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
19	1V	101/103 (98%)	97 (96%)	3 (3%)	1 (1%)	12	45
20	1W	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
21	1X	91/100 (91%)	87 (96%)	3 (3%)	1 (1%)	11	43
22	1Y	100/104 (96%)	96 (96%)	3 (3%)	1 (1%)	12	45
23	1Z	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
24	10	75/85 (88%)	74 (99%)	1 (1%)	0	100	100
25	11	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
26	12	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
27	13	57/59 (97%)	55 (96%)	1 (2%)	1 (2%)	6	34
28	15	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
29	16	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
30	17	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
31	18	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
32	19	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
34	1b	216/241 (90%)	189 (88%)	19 (9%)	8 (4%)	2	21
35	1c	204/233 (88%)	180 (88%)	19 (9%)	5 (2%)	4	28
36	1d	203/206 (98%)	187 (92%)	8 (4%)	8 (4%)	2	20
37	1e	148/167 (89%)	124 (84%)	17 (12%)	7 (5%)	2	17
38	1f	98/135 (73%)	84 (86%)	10 (10%)	4 (4%)	2	19
39	1g	149/179 (83%)	141 (95%)	7 (5%)	1 (1%)	18	51
40	1h	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
41	1i	125/130 (96%)	113 (90%)	6 (5%)	6 (5%)	2	16
42	1j	96/103 (93%)	83 (86%)	7 (7%)	6 (6%)	1	12
43	1k	115/129 (89%)	99 (86%)	13 (11%)	3 (3%)	4	27
44	1l	121/124 (98%)	106 (88%)	9 (7%)	6 (5%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	1m	112/118 (95%)	102 (91%)	9 (8%)	1 (1%)	14	46
46	1n	92/101 (91%)	79 (86%)	8 (9%)	5 (5%)	1	14
47	1o	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
48	1p	80/82 (98%)	68 (85%)	10 (12%)	2 (2%)	4	28
49	1q	78/84 (93%)	62 (80%)	12 (15%)	4 (5%)	1	15
50	1r	53/75 (71%)	52 (98%)	1 (2%)	0	100	100
51	1s	77/92 (84%)	72 (94%)	4 (5%)	1 (1%)	9	39
52	1t	83/87 (95%)	77 (93%)	4 (5%)	2 (2%)	4	29
53	1u	49/71 (69%)	36 (74%)	8 (16%)	5 (10%)	0	5
All	All	5755/6150 (94%)	5333 (93%)	326 (6%)	96 (2%)	9	35

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	1K	15	ALA
10	1K	19	ASN
14	1Q	51	ARG
22	1Y	52	LEU
36	1d	30	THR
37	1e	105	ILE
41	1i	55	VAL
41	1i	91	ASP
41	1i	129	LYS
43	1k	127	ARG
44	1l	34	CYS
46	1n	92	GLU
49	1q	51	ASN
53	1u	9	ASN
53	1u	40	LYS
8	1I	118	PRO
9	1J	67	THR
9	1J	106	PHE
9	1J	108	VAL
10	1K	23	PRO
10	1K	25	GLY
12	1O	108	ARG
14	1Q	52	ALA
19	1V	44	GLY
34	1b	82	ASP

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Mol	Chain	Res	Type
34	1b	193	PRO
35	1c	206	GLU
36	1d	28	ILE
37	1e	12	GLN
37	1e	122	ASN
37	1e	158	GLY
39	1g	114	LYS
41	1i	9	THR
41	1i	13	LYS
41	1i	58	VAL
42	1j	57	VAL
43	1k	89	PRO
44	1l	23	ALA
44	1l	24	LEU
44	1l	76	GLU
45	1m	114	LYS
48	1p	43	ALA
49	1q	17	MET
52	1t	41	ALA
53	1u	24	GLU
9	1J	104	ALA
17	1T	105	GLY
27	13	4	THR
34	1b	68	LEU
36	1d	153	SER
36	1d	165	ARG
36	1d	175	ALA
37	1e	24	THR
38	1f	54	LEU
38	1f	86	ARG
42	1j	95	GLY
46	1n	22	ALA
51	1s	5	LEU
53	1u	10	GLU
34	1b	19	GLN
34	1b	75	ALA
35	1c	80	LYS
35	1c	166	GLU
36	1d	192	SER
36	1d	193	ALA
37	1e	101	GLU
38	1f	63	ASN

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Mol	Chain	Res	Type
44	1l	43	LYS
44	1l	78	SER
46	1n	3	LYS
48	1p	47	GLU
49	1q	76	VAL
53	1u	35	ARG
3	1D	253	LYS
8	1I	122	LEU
15	1R	106	ASP
34	1b	34	ALA
34	1b	149	GLY
34	1b	168	HIS
36	1d	167	LYS
38	1f	94	HIS
42	1j	36	VAL
46	1n	52	PRO
49	1q	80	GLU
52	1t	68	HIS
9	1J	130	PRO
42	1j	41	PRO
42	1j	42	LEU
21	1X	90	GLY
35	1c	66	VAL
37	1e	143	GLY
42	1j	100	ILE
9	1J	88	HIS
35	1c	81	GLY
43	1k	92	GLY
46	1n	34	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	216/218 (99%)	216 (100%)	0	100	100
4	1E	163/163 (100%)	163 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	1F	165/165 (100%)	165 (100%)	0	100	100
6	1G	147/150 (98%)	145 (99%)	2 (1%)	59	71
7	1H	137/138 (99%)	136 (99%)	1 (1%)	76	78
8	1I	114/114 (100%)	114 (100%)	0	100	100
9	1J	103/123 (84%)	102 (99%)	1 (1%)	68	75
10	1K	104/110 (94%)	104 (100%)	0	100	100
11	1N	116/116 (100%)	114 (98%)	2 (2%)	53	69
12	1O	104/104 (100%)	104 (100%)	0	100	100
13	1P	103/103 (100%)	103 (100%)	0	100	100
14	1Q	111/109 (102%)	106 (96%)	5 (4%)	24	51
15	1R	102/103 (99%)	101 (99%)	1 (1%)	68	75
16	1S	87/87 (100%)	87 (100%)	0	100	100
17	1T	99/100 (99%)	98 (99%)	1 (1%)	68	75
18	1U	89/90 (99%)	88 (99%)	1 (1%)	65	74
19	1V	84/84 (100%)	84 (100%)	0	100	100
20	1W	93/93 (100%)	93 (100%)	0	100	100
21	1X	80/84 (95%)	80 (100%)	0	100	100
22	1Y	83/85 (98%)	83 (100%)	0	100	100
23	1Z	78/78 (100%)	78 (100%)	0	100	100
24	10	58/63 (92%)	56 (97%)	2 (3%)	32	57
25	11	67/68 (98%)	67 (100%)	0	100	100
26	12	54/55 (98%)	54 (100%)	0	100	100
27	13	49/49 (100%)	49 (100%)	0	100	100
28	15	47/48 (98%)	46 (98%)	1 (2%)	47	65
29	16	45/49 (92%)	45 (100%)	0	100	100
30	17	38/38 (100%)	38 (100%)	0	100	100
31	18	51/52 (98%)	51 (100%)	0	100	100
32	19	34/34 (100%)	34 (100%)	0	100	100
34	1b	180/199 (90%)	180 (100%)	0	100	100
35	1c	170/190 (90%)	170 (100%)	0	100	100
36	1d	172/173 (99%)	171 (99%)	1 (1%)	78	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	1e	113/126 (90%)	112 (99%)	1 (1%)	70	76
38	1f	87/116 (75%)	87 (100%)	0	100	100
39	1g	124/147 (84%)	124 (100%)	0	100	100
40	1h	104/105 (99%)	104 (100%)	0	100	100
41	1i	105/107 (98%)	105 (100%)	0	100	100
42	1j	86/90 (96%)	86 (100%)	0	100	100
43	1k	90/99 (91%)	90 (100%)	0	100	100
44	1l	103/104 (99%)	103 (100%)	0	100	100
45	1m	92/96 (96%)	91 (99%)	1 (1%)	65	74
46	1n	79/84 (94%)	79 (100%)	0	100	100
47	1o	75/77 (97%)	75 (100%)	0	100	100
48	1p	65/65 (100%)	65 (100%)	0	100	100
49	1q	74/78 (95%)	74 (100%)	0	100	100
50	1r	48/65 (74%)	48 (100%)	0	100	100
51	1s	70/79 (89%)	70 (100%)	0	100	100
52	1t	65/66 (98%)	65 (100%)	0	100	100
53	1u	44/61 (72%)	44 (100%)	0	100	100
All	All	4767/5000 (95%)	4747 (100%)	20 (0%)	81	81

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	1G	67	ILE
6	1G	154	ILE
7	1H	43	VAL
9	1J	82	ILE
11	1N	136	GLN
11	1N	142	ILE
14	1Q	54	THR
14	1Q	55	ARG
14	1Q	58	LYS
14	1Q	59	ARG
14	1Q	60	GLN
15	1R	33	ILE
17	1T	106	LYS
18	1U	41	LYS

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Mol	Chain	Res	Type
24	10	23	VAL
24	10	66	LYS
28	15	57	LYS
36	1d	191	LEU
37	1e	11	LEU
45	1m	25	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	90	ASN
3	1D	153	GLN
3	1D	200	HIS
4	1E	32	ASN
4	1E	49	GLN
4	1E	130	GLN
4	1E	173	GLN
5	1F	92	HIS
5	1F	165	HIS
6	1G	27	GLN
6	1G	37	ASN
6	1G	63	GLN
7	1H	88	GLN
8	1I	2	GLN
8	1I	66	ASN
8	1I	145	ASN
10	1K	30	GLN
10	1K	31	GLN
10	1K	94	ASN
11	1N	47	HIS
11	1N	80	HIS
12	1O	93	GLN
13	1P	35	HIS
13	1P	54	GLN
14	1Q	13	HIS
15	1R	31	HIS
15	1R	73	ASN
16	1S	29	HIS
16	1S	98	GLN
16	1S	100	HIS
17	1T	12	GLN
17	1T	56	HIS

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Mol	Chain	Res	Type
18	1U	37	GLN
18	1U	44	GLN
19	1V	89	HIS
20	1W	40	ASN
21	1X	92	ASN
24	10	57	HIS
25	11	17	ASN
25	11	34	HIS
25	11	36	HIS
27	13	20	HIS
28	15	42	HIS
29	16	19	HIS
31	18	24	HIS
31	18	26	HIS
32	19	13	ASN
34	1b	15	HIS
35	1c	102	ASN
35	1c	190	HIS
36	1d	116	GLN
36	1d	136	GLN
36	1d	152	GLN
38	1f	37	HIS
38	1f	55	HIS
39	1g	28	ASN
39	1g	148	ASN
40	1h	4	GLN
40	1h	16	ASN
40	1h	76	GLN
42	1j	58	ASN
43	1k	118	HIS
43	1k	119	ASN
44	1l	5	ASN
44	1l	77	HIS
46	1n	43	ASN
47	1o	50	HIS
48	1p	18	GLN
48	1p	63	GLN
49	1q	31	HIS
50	1r	52	GLN
51	1s	57	HIS
51	1s	69	HIS
52	1t	48	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2887/2904 (99%)	360 (12%)	10 (0%)
2	1B	119/120 (99%)	8 (6%)	0
33	1a	1538/1539 (99%)	227 (14%)	0
54	1v	2/9 (22%)	0	0
55	1x	86/87 (98%)	22 (25%)	0
All	All	4632/4659 (99%)	617 (13%)	10 (0%)

All (617) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	A
1	1A	12	U
1	1A	15	G
1	1A	34	U
1	1A	46	G
1	1A	63	A
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	80	G
1	1A	101	A
1	1A	102	U
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	135	U
1	1A	136	G
1	1A	137	U
1	1A	138	U
1	1A	139	U
1	1A	140	C
1	1A	141	G
1	1A	142	A
1	1A	196	A
1	1A	199	A
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	248	G
1	1A	266	G
1	1A	272	A

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Mol	Chain	Res	Type
1	1A	276	U
1	1A	277	G
1	1A	279	A
1	1A	283	G
1	1A	285	G
1	1A	291	G
1	1A	302	C
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	331	C
1	1A	353	C
1	1A	358	U
1	1A	361	G
1	1A	362	A
1	1A	370	G
1	1A	372	G
1	1A	383	C
1	1A	386	G
1	1A	396	G
1	1A	411	G
1	1A	412	A
1	1A	424	G
1	1A	425	G
1	1A	435	C
1	1A	451	U
1	1A	481	G
1	1A	491	G
1	1A	504	A
1	1A	505	A
1	1A	508	A
1	1A	531	C
1	1A	532	A
1	1A	543	G
1	1A	546	U
1	1A	547	A
1	1A	548	G
1	1A	549	G
1	1A	550	C
1	1A	551	G
1	1A	563	A
1	1A	573	U

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Mol	Chain	Res	Type
1	1A	575	A
1	1A	603	A
1	1A	613	A
1	1A	614	A
1	1A	615	U
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	647	G
1	1A	654	A
1	1A	686	U
1	1A	730	A
1	1A	747	5MU
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	G
1	1A	785	G
1	1A	790	U
1	1A	792	A
1	1A	805	G
1	1A	812	C
1	1A	827	U
1	1A	828	U
1	1A	845	A
1	1A	846	U
1	1A	847	U
1	1A	858	G
1	1A	859	G
1	1A	866	A
1	1A	878	A
1	1A	885	C
1	1A	893	C
1	1A	896	A
1	1A	897	C
1	1A	910	A
1	1A	914	G
1	1A	915	C
1	1A	931	U
1	1A	946	C
1	1A	961	C
1	1A	974	G

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Mol	Chain	Res	Type
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	G
1	1A	1033	U
1	1A	1046	A
1	1A	1047	G
1	1A	1070	A
1	1A	1083	U
1	1A	1088	A
1	1A	1090	A
1	1A	1112	G
1	1A	1128	G
1	1A	1130	U
1	1A	1132	U
1	1A	1133	A
1	1A	1135	C
1	1A	1136	G
1	1A	1142	A
1	1A	1168	G
1	1A	1171	G
1	1A	1172	C
1	1A	1175	A
1	1A	1176	U
1	1A	1177	G
1	1A	1182	G
1	1A	1238	G
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	G
1	1A	1301	A
1	1A	1352	U
1	1A	1365	A
1	1A	1379	U
1	1A	1383	A
1	1A	1416	G
1	1A	1417	C

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Mol	Chain	Res	Type
1	1A	1428	C
1	1A	1452	G
1	1A	1453	A
1	1A	1482	G
1	1A	1490	A
1	1A	1493	C
1	1A	1494	A
1	1A	1495	A
1	1A	1497	U
1	1A	1510	G
1	1A	1515	A
1	1A	1523	U
1	1A	1532	A
1	1A	1533	C
1	1A	1535	A
1	1A	1536	C
1	1A	1537	G
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1581	G
1	1A	1583	A
1	1A	1584	U
1	1A	1585	C
1	1A	1606	C
1	1A	1607	C
1	1A	1608	A
1	1A	1647	U
1	1A	1648	U
1	1A	1649	G
1	1A	1674	G
1	1A	1714	U
1	1A	1715	G
1	1A	1725	U
1	1A	1727	C
1	1A	1729	U
1	1A	1730	C
1	1A	1731	G
1	1A	1738	G
1	1A	1740	G
1	1A	1744	A
1	1A	1755	A

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Mol	Chain	Res	Type
1	1A	1764	C
1	1A	1773	A
1	1A	1782	U
1	1A	1800	C
1	1A	1801	A
1	1A	1808	A
1	1A	1816	C
1	1A	1829	A
1	1A	1858	A
1	1A	1859	U
1	1A	1870	C
1	1A	1871	A
1	1A	1872	A
1	1A	1873	G
1	1A	1876	A
1	1A	1906	G
1	1A	1907	G
1	1A	1913	A
1	1A	1914	C
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1967	C
1	1A	1970	A
1	1A	1972	G
1	1A	1991	U
1	1A	1993	U
1	1A	1997	C
1	1A	2023	C
1	1A	2031	A
1	1A	2033	A
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G7M
1	1A	2070	A
1	1A	2093	G

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Mol	Chain	Res	Type
1	1A	2097	A
1	1A	2101	A
1	1A	2105	U
1	1A	2108	A
1	1A	2111	U
1	1A	2112	G
1	1A	2113	U
1	1A	2115	G
1	1A	2116	G
1	1A	2117	A
1	1A	2118	U
1	1A	2119	A
1	1A	2121	G
1	1A	2123	G
1	1A	2126	A
1	1A	2128	G
1	1A	2131	U
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2136	G
1	1A	2137	U
1	1A	2145	C
1	1A	2146	C
1	1A	2147	A
1	1A	2148	G
1	1A	2149	U
1	1A	2159	G
1	1A	2160	C
1	1A	2161	C
1	1A	2162	G
1	1A	2163	A
1	1A	2164	C
1	1A	2165	C
1	1A	2167	U
1	1A	2168	G
1	1A	2169	A
1	1A	2170	A
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2177	C

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Mol	Chain	Res	Type
1	1A	2178	C
1	1A	2179	C
1	1A	2181	U
1	1A	2185	U
1	1A	2187	U
1	1A	2188	U
1	1A	2190	G
1	1A	2198	A
1	1A	2204	G
1	1A	2211	A
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2273	A
1	1A	2283	C
1	1A	2286	G
1	1A	2287	A
1	1A	2305	U
1	1A	2308	G
1	1A	2324	U
1	1A	2325	G
1	1A	2327	A
1	1A	2333	A
1	1A	2335	A
1	1A	2339	C
1	1A	2347	C
1	1A	2383	G
1	1A	2385	C
1	1A	2406	A
1	1A	2424	C
1	1A	2425	A
1	1A	2435	A
1	1A	2441	U
1	1A	2448	A
1	1A	2476	A
1	1A	2491	U
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2529	G
1	1A	2547	A

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Mol	Chain	Res	Type
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2585	U
1	1A	2586	U
1	1A	2603	G
1	1A	2609	U
1	1A	2613	U
1	1A	2629	U
1	1A	2663	G
1	1A	2682	A
1	1A	2689	U
1	1A	2690	U
1	1A	2714	G
1	1A	2726	A
1	1A	2744	G
1	1A	2748	A
1	1A	2765	A
1	1A	2778	A
1	1A	2791	G
1	1A	2792	A
1	1A	2798	U
1	1A	2799	A
1	1A	2811	G
1	1A	2818	U
1	1A	2820	A
1	1A	2821	A
1	1A	2825	G
1	1A	2836	U
1	1A	2867	G
1	1A	2873	A
1	1A	2874	C
1	1A	2880	C
1	1A	2883	A
1	1A	2891	U
2	1B	25	U
2	1B	35	C
2	1B	45	A
2	1B	56	G
2	1B	66	A
2	1B	89	U
2	1B	90	C

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Mol	Chain	Res	Type
2	1B	109	A
33	1a	5	U
33	1a	7	A
33	1a	9	G
33	1a	32	A
33	1a	39	G
33	1a	47	C
33	1a	48	C
33	1a	51	A
33	1a	70	U
33	1a	71	A
33	1a	74	A
33	1a	83	C
33	1a	85	U
33	1a	87	C
33	1a	88	U
33	1a	95	C
33	1a	97	G
33	1a	108	G
33	1a	116	A
33	1a	120	A
33	1a	121	U
33	1a	122	G
33	1a	130	A
33	1a	131	A
33	1a	149	A
33	1a	164	G
33	1a	182	A
33	1a	183	C
33	1a	204	G
33	1a	207	C
33	1a	208	U
33	1a	210	C
33	1a	211	G
33	1a	212	G
33	1a	247	G
33	1a	251	G
33	1a	266	G
33	1a	267	C
33	1a	279	A
33	1a	280	C
33	1a	289	G

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Mol	Chain	Res	Type
33	1a	298	A
33	1a	321	A
33	1a	328	C
33	1a	329	A
33	1a	330	C
33	1a	332	G
33	1a	347	G
33	1a	352	C
33	1a	354	G
33	1a	356	A
33	1a	367	U
33	1a	372	C
33	1a	378	G
33	1a	397	A
33	1a	406	G
33	1a	411	A
33	1a	412	A
33	1a	413	G
33	1a	421	U
33	1a	422	C
33	1a	424	G
33	1a	429	U
33	1a	430	A
33	1a	451	A
33	1a	452	A
33	1a	459	A
33	1a	467	U
33	1a	468	A
33	1a	478	A
33	1a	479	U
33	1a	481	G
33	1a	485	U
33	1a	486	U
33	1a	496	A
33	1a	497	G
33	1a	509	A
33	1a	511	C
33	1a	518	C
33	1a	527	G
33	1a	532	A
33	1a	547	A
33	1a	559	A

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Mol	Chain	Res	Type
33	1a	563	A
33	1a	564	C
33	1a	571	U
33	1a	572	A
33	1a	573	A
33	1a	576	C
33	1a	577	G
33	1a	596	A
33	1a	633	G
33	1a	642	A
33	1a	650	G
33	1a	665	A
33	1a	687	A
33	1a	695	A
33	1a	702	A
33	1a	703	G
33	1a	721	G
33	1a	723	U
33	1a	731	G
33	1a	733	G
33	1a	747	A
33	1a	755	G
33	1a	777	A
33	1a	787	A
33	1a	792	A
33	1a	793	U
33	1a	794	A
33	1a	814	A
33	1a	815	A
33	1a	817	C
33	1a	828	U
33	1a	829	G
33	1a	832	G
33	1a	841	C
33	1a	842	U
33	1a	843	U
33	1a	844	G
33	1a	845	A
33	1a	846	G
33	1a	873	A
33	1a	880	C
33	1a	885	G

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Mol	Chain	Res	Type
33	1a	900	A
33	1a	914	A
33	1a	926	G
33	1a	934	C
33	1a	935	A
33	1a	960	U
33	1a	969	A
33	1a	971	G
33	1a	975	A
33	1a	976	G
33	1a	977	A
33	1a	983	A
33	1a	993	G
33	1a	1004	A
33	1a	1008	U
33	1a	1018	G
33	1a	1026	G
33	1a	1027	C
33	1a	1030	U
33	1a	1031	C
33	1a	1032	G
33	1a	1033	G
33	1a	1034	G
33	1a	1036	A
33	1a	1043	G
33	1a	1044	A
33	1a	1050	G
33	1a	1054	C
33	1a	1065	U
33	1a	1073	U
33	1a	1088	G
33	1a	1094	G
33	1a	1095	U
33	1a	1101	A
33	1a	1125	U
33	1a	1133	G
33	1a	1134	G
33	1a	1136	C
33	1a	1137	C
33	1a	1139	G
33	1a	1140	C
33	1a	1141	C

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Mol	Chain	Res	Type
33	1a	1142	G
33	1a	1145	A
33	1a	1152	A
33	1a	1159	U
33	1a	1160	G
33	1a	1161	C
33	1a	1168	U
33	1a	1184	G
33	1a	1196	A
33	1a	1197	A
33	1a	1201	A
33	1a	1202	U
33	1a	1212	U
33	1a	1213	A
33	1a	1227	A
33	1a	1236	A
33	1a	1238	A
33	1a	1240	U
33	1a	1241	G
33	1a	1253	G
33	1a	1256	A
33	1a	1257	A
33	1a	1261	A
33	1a	1275	A
33	1a	1280	A
33	1a	1285	A
33	1a	1286	U
33	1a	1287	A
33	1a	1293	C
33	1a	1299	A
33	1a	1300	G
33	1a	1302	C
33	1a	1305	G
33	1a	1317	C
33	1a	1318	A
33	1a	1322	C
33	1a	1337	G
33	1a	1346	A
33	1a	1347	G
33	1a	1363	A
33	1a	1364	U
33	1a	1379	G

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Mol	Chain	Res	Type
33	1a	1398	A
33	1a	1429	A
33	1a	1441	A
33	1a	1446	A
33	1a	1492	A
33	1a	1493	A
33	1a	1499	A
33	1a	1503	A
33	1a	1505	G
33	1a	1506	U
33	1a	1507	A
33	1a	1517	G
33	1a	1519	A
33	1a	1529	G
33	1a	1530	G
33	1a	1533	C
33	1a	1535	C
33	1a	1536	C
55	1x	7	G
55	1x	8	U
55	1x	9	G
55	1x	14	A
55	1x	16	U
55	1x	17	U
55	1x	18	G
55	1x	19	G
55	1x	20	U
55	1x	21	A
55	1x	22	G
55	1x	23	A
55	1x	24	C
55	1x	27	G
55	1x	46	G
55	1x	49	C
55	1x	50	A
55	1x	58	U
55	1x	68	A
55	1x	79	U
55	1x	86	C
55	1x	87	A

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	784	G
1	1A	1494	A
1	1A	1730	C
1	1A	2118	U
1	1A	2127	G
1	1A	2158	A
1	1A	2324	U
1	1A	2406	A
1	1A	2585	U
1	1A	2873	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

26 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	1A	2251	1,55	23,26,27	1.19	3 (13%)	32,38,41	1.98	6 (18%)
1	PSU	1A	1917	1	18,21,22	1.42	2 (11%)	21,30,33	2.20	4 (19%)
1	PSU	1A	2504	1	18,21,22	1.40	2 (11%)	21,30,33	2.06	4 (19%)
1	6MZ	1A	1618	1	22,25,26	1.49	4 (18%)	29,36,39	2.17	9 (31%)
1	PSU	1A	2580	1	18,21,22	1.39	3 (16%)	21,30,33	2.12	5 (23%)
1	1MG	1A	745	1	23,26,27	1.21	3 (13%)	33,39,42	1.73	5 (15%)
1	5MU	1A	747	1	19,22,23	1.37	5 (26%)	27,32,35	2.12	6 (22%)
1	PSU	1A	746	1	18,21,22	1.42	2 (11%)	21,30,33	2.06	4 (19%)
1	PSU	1A	2457	1	18,21,22	1.42	2 (11%)	21,30,33	2.16	5 (23%)
1	PSU	1A	1911	1	18,21,22	1.37	2 (11%)	21,30,33	2.09	4 (19%)
4	MEQ	1E	150[B]	4	8,9,10	0.65	0	5,10,12	0.52	0
1	PSU	1A	2604	1	18,21,22	1.37	2 (11%)	21,30,33	2.00	4 (19%)
1	PSU	1A	1915	1	18,21,22	1.37	2 (11%)	21,30,33	2.12	4 (19%)
1	PSU	1A	2605	1	18,21,22	1.39	3 (16%)	21,30,33	2.18	4 (19%)
1	2MG	1A	2445	1	23,26,27	1.22	2 (8%)	33,38,41	2.18	9 (27%)
1	2MA	1A	2503	1	22,25,26	1.50	5 (22%)	32,37,40	2.11	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	G7M	1A	2069	1	23,26,27	1.96	3 (13%)	34,39,42	2.37	12 (35%)
1	5MU	1A	1939	1	19,22,23	1.43	6 (31%)	27,32,35	2.14	6 (22%)
1	5MC	1A	1962	1	19,22,23	1.66	3 (15%)	26,32,35	1.06	2 (7%)
1	PSU	1A	955	1	18,21,22	1.38	2 (11%)	21,30,33	2.24	4 (19%)
1	2MG	1A	1835	1	23,26,27	1.27	4 (17%)	33,38,41	2.16	6 (18%)
1	OMC	1A	2498	1	19,22,23	0.79	0	25,31,34	1.04	1 (4%)
1	OMU	1A	2552	1	19,22,23	1.22	2 (10%)	25,31,34	1.82	5 (20%)
1	6MZ	1A	2030	1	22,25,26	1.46	5 (22%)	29,36,39	2.41	10 (34%)
1	H2U	1A	2449	1	18,21,22	1.01	2 (11%)	19,30,33	1.11	3 (15%)
4	MEQ	1E	150[A]	4	8,9,10	0.60	0	5,10,12	0.72	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	1A	2251	1,55	-	0/9/27/28	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2504	1	-	1/7/25/26	0/2/2/2
1	6MZ	1A	1618	1	-	0/9/27/28	0/3/3/3
1	PSU	1A	2580	1	-	0/7/25/26	0/2/2/2
1	1MG	1A	745	1	-	0/7/25/26	0/3/3/3
1	5MU	1A	747	1	-	1/7/25/26	0/2/2/2
1	PSU	1A	746	1	-	4/7/25/26	0/2/2/2
1	PSU	1A	2457	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
4	MEQ	1E	150[B]	4	-	4/8/9/11	-
1	PSU	1A	2604	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1915	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	2MG	1A	2445	1	-	1/9/27/28	0/3/3/3
1	2MA	1A	2503	1	-	2/7/25/26	0/3/3/3
1	G7M	1A	2069	1	-	1/7/25/26	0/3/3/3
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1	-	2/7/25/26	0/2/2/2
1	PSU	1A	955	1	-	0/7/25/26	0/2/2/2
1	2MG	1A	1835	1	-	2/9/27/28	0/3/3/3
1	OMC	1A	2498	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	1A	2552	1	-	0/9/27/28	0/2/2/2
1	6MZ	1A	2030	1	-	2/9/27/28	0/3/3/3
1	H2U	1A	2449	1	-	0/7/38/39	0/2/2/2
4	MEQ	1E	150[A]	4	-	2/8/9/11	-

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2069	G7M	C5-N7	-7.58	1.30	1.39
1	1A	1962	5MC	C5-C4	6.04	1.48	1.44
1	1A	1618	6MZ	C5-C4	4.79	1.47	1.39
1	1A	2503	2MA	C5-C4	4.64	1.47	1.39
1	1A	2030	6MZ	C5-C4	4.32	1.46	1.39
1	1A	2457	PSU	C6-C5	3.67	1.39	1.35
1	1A	1917	PSU	C6-C5	3.67	1.39	1.35
1	1A	2504	PSU	C6-C5	3.58	1.39	1.35
1	1A	2604	PSU	C6-C5	3.53	1.39	1.35
1	1A	746	PSU	C6-C5	3.37	1.39	1.35
1	1A	2605	PSU	C6-C5	3.37	1.39	1.35
1	1A	1911	PSU	C6-C5	3.34	1.39	1.35
1	1A	955	PSU	C6-C5	3.28	1.38	1.35
1	1A	1915	PSU	C6-C5	3.27	1.38	1.35
1	1A	745	1MG	C5-C4	3.23	1.47	1.38
1	1A	2251	OMG	C5-C4	3.17	1.47	1.38
1	1A	1835	2MG	C5-C4	3.14	1.47	1.38
1	1A	2445	2MG	C5-C4	3.04	1.47	1.38
1	1A	2580	PSU	C6-C5	3.03	1.38	1.35
1	1A	1962	5MC	C6-C5	2.85	1.39	1.34
1	1A	2069	G7M	C4-N9	-2.85	1.30	1.38
1	1A	1939	5MU	C6-C5	2.82	1.39	1.34
1	1A	2605	PSU	C4-N3	-2.80	1.33	1.38
1	1A	2030	6MZ	C5-C6	2.78	1.48	1.41
1	1A	2580	PSU	C4-N3	-2.77	1.33	1.38
1	1A	1939	5MU	C4-N3	-2.76	1.33	1.38
1	1A	1917	PSU	C4-N3	-2.76	1.33	1.38
1	1A	2069	G7M	C6-N1	-2.76	1.33	1.38
1	1A	1911	PSU	C4-N3	-2.73	1.33	1.38
1	1A	746	PSU	C4-N3	-2.72	1.33	1.38
1	1A	2457	PSU	C4-N3	-2.72	1.33	1.38
1	1A	2604	PSU	C4-N3	-2.70	1.33	1.38
1	1A	747	5MU	C6-C5	2.67	1.39	1.34
1	1A	955	PSU	C4-N3	-2.67	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2449	H2U	C2-N3	-2.65	1.33	1.38
1	1A	1915	PSU	C4-N3	-2.64	1.33	1.38
1	1A	1618	6MZ	C5-C6	2.62	1.48	1.41
1	1A	2552	OMU	C4-N3	-2.62	1.34	1.38
1	1A	2504	PSU	C4-N3	-2.61	1.34	1.38
1	1A	2503	2MA	C5-C6	2.57	1.48	1.41
1	1A	1835	2MG	C6-N1	-2.57	1.34	1.38
1	1A	747	5MU	C4-N3	-2.55	1.34	1.38
1	1A	745	1MG	C2-N1	2.55	1.41	1.37
1	1A	2449	H2U	C4-N3	-2.54	1.33	1.37
1	1A	1939	5MU	C4-C5	2.46	1.48	1.44
1	1A	2030	6MZ	C8-N7	2.45	1.36	1.31
1	1A	2503	2MA	C8-N7	2.43	1.36	1.31
1	1A	2445	2MG	C6-N1	-2.40	1.34	1.38
1	1A	1618	6MZ	C8-N7	2.38	1.36	1.31
1	1A	1618	6MZ	C5-N7	-2.38	1.34	1.39
1	1A	2251	OMG	C6-N1	-2.38	1.34	1.38
1	1A	747	5MU	C4-C5	2.37	1.48	1.44
1	1A	1939	5MU	C6-N1	-2.34	1.34	1.38
1	1A	747	5MU	C6-N1	-2.32	1.34	1.38
1	1A	2503	2MA	C5-N7	-2.31	1.34	1.39
1	1A	1835	2MG	C2-N3	2.27	1.36	1.32
1	1A	745	1MG	C5-N7	-2.18	1.34	1.39
1	1A	2030	6MZ	C4-N9	-2.16	1.33	1.37
1	1A	2030	6MZ	C5-N7	-2.15	1.35	1.39
1	1A	2503	2MA	C4-N9	-2.14	1.33	1.37
1	1A	2552	OMU	C2-N3	-2.11	1.34	1.38
1	1A	1939	5MU	C2-N3	-2.10	1.34	1.38
1	1A	2251	OMG	C5-N7	-2.08	1.34	1.39
1	1A	1835	2MG	C5-N7	-2.07	1.34	1.39
1	1A	1962	5MC	C6-N1	-2.05	1.34	1.38
1	1A	2580	PSU	O4'-C1'	-2.04	1.41	1.43
1	1A	2605	PSU	C2-N3	-2.04	1.34	1.37
1	1A	747	5MU	C2-N1	2.02	1.41	1.38
1	1A	1939	5MU	C2-N1	2.01	1.41	1.38

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1835	2MG	C2-N3-C4	7.08	120.86	112.00
1	1A	2445	2MG	C2-N3-C4	6.97	120.72	112.00
1	1A	2503	2MA	C5-C4-N3	-6.97	119.84	127.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1917	PSU	N1-C2-N3	6.94	122.49	115.17
1	1A	955	PSU	N1-C2-N3	6.85	122.40	115.17
1	1A	2457	PSU	N1-C2-N3	6.79	122.33	115.17
1	1A	2605	PSU	N1-C2-N3	6.68	122.21	115.17
1	1A	1915	PSU	N1-C2-N3	6.59	122.12	115.17
1	1A	746	PSU	N1-C2-N3	6.53	122.06	115.17
1	1A	1911	PSU	N1-C2-N3	6.45	121.97	115.17
1	1A	2580	PSU	N1-C2-N3	6.42	121.94	115.17
1	1A	2251	OMG	C5-C4-N3	-6.22	118.49	128.39
1	1A	1835	2MG	C5-C4-N3	-6.21	118.51	128.39
1	1A	2504	PSU	N1-C2-N3	6.20	121.70	115.17
1	1A	2604	PSU	N1-C2-N3	6.19	121.69	115.17
1	1A	2069	G7M	C2'-C1'-N9	-6.01	96.53	113.25
1	1A	1618	6MZ	C5-C4-N3	-5.80	118.74	126.72
1	1A	2445	2MG	C5-C4-N3	-5.68	119.35	128.39
1	1A	2030	6MZ	C5-C4-N3	-5.54	119.09	126.72
1	1A	2503	2MA	N3-C4-N9	5.49	133.96	126.99
1	1A	745	1MG	C5-C4-N3	-5.49	119.66	128.39
1	1A	2069	G7M	C5-C4-N3	-5.42	117.92	128.15
1	1A	2069	G7M	N9-C4-N3	5.41	136.78	125.95
1	1A	1939	5MU	C4-N3-C2	-5.38	120.28	127.34
1	1A	1939	5MU	N3-C2-N1	5.34	121.84	114.89
1	1A	2251	OMG	C2-N3-C4	5.18	121.22	112.30
1	1A	747	5MU	C4-N3-C2	-5.17	120.57	127.34
1	1A	747	5MU	N3-C2-N1	5.15	121.60	114.89
1	1A	2069	G7M	C2-N3-C4	5.03	120.97	112.30
1	1A	2552	OMU	C4-N3-C2	-4.93	120.50	126.61
1	1A	955	PSU	C4-N3-C2	-4.64	119.98	126.37
1	1A	1835	2MG	N9-C4-N3	4.59	135.13	125.95
1	1A	2605	PSU	C4-N3-C2	-4.59	120.05	126.37
1	1A	2030	6MZ	C9-N6-C6	-4.56	118.62	122.85
1	1A	2251	OMG	N9-C4-N3	4.47	134.89	125.95
1	1A	955	PSU	O2-C2-N1	-4.47	118.18	122.79
1	1A	2030	6MZ	C6-C5-N7	4.46	137.30	132.43
1	1A	1915	PSU	C4-N3-C2	-4.43	120.27	126.37
1	1A	1618	6MZ	N3-C4-N9	4.43	134.70	127.17
1	1A	746	PSU	C4-N3-C2	-4.39	120.32	126.37
1	1A	2580	PSU	C4-N3-C2	-4.39	120.33	126.37
1	1A	2457	PSU	C4-N3-C2	-4.35	120.38	126.37
1	1A	1917	PSU	C4-N3-C2	-4.32	120.42	126.37
1	1A	1939	5MU	C5-C4-N3	4.31	119.07	115.32
1	1A	1911	PSU	C4-N3-C2	-4.27	120.49	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2552	OMU	N3-C2-N1	4.24	120.42	114.89
1	1A	1917	PSU	O2-C2-N1	-4.20	118.45	122.79
1	1A	745	1MG	C2-N3-C4	4.19	121.39	111.98
1	1A	2030	6MZ	N3-C4-N9	4.14	134.21	127.17
1	1A	2604	PSU	C4-N3-C2	-4.10	120.72	126.37
1	1A	747	5MU	C5-C4-N3	4.09	118.88	115.32
1	1A	2504	PSU	C4-N3-C2	-4.09	120.74	126.37
1	1A	745	1MG	N9-C4-N3	4.04	134.04	125.95
1	1A	2504	PSU	O2-C2-N1	-4.04	118.62	122.79
1	1A	2030	6MZ	C4-C5-N7	-4.04	105.97	110.58
1	1A	2445	2MG	N9-C4-N3	4.03	134.02	125.95
1	1A	1939	5MU	C5-C6-N1	-4.03	118.94	123.31
1	1A	1618	6MZ	C9-N6-C6	-4.02	119.12	122.85
1	1A	2552	OMU	C5-C4-N3	3.95	120.34	114.80
1	1A	1911	PSU	O2-C2-N1	-3.94	118.72	122.79
1	1A	2457	PSU	O2-C2-N1	-3.88	118.79	122.79
1	1A	2605	PSU	O2-C2-N1	-3.85	118.82	122.79
1	1A	2030	6MZ	C2-N3-C4	3.76	121.01	111.83
1	1A	747	5MU	O4-C4-C5	-3.72	120.66	124.92
1	1A	1915	PSU	O2-C2-N1	-3.65	119.03	122.79
1	1A	2580	PSU	O2-C2-N1	-3.64	119.04	122.79
1	1A	1618	6MZ	C2-N3-C4	3.56	120.52	111.83
1	1A	1939	5MU	O4-C4-C5	-3.55	120.86	124.92
1	1A	747	5MU	C5-C6-N1	-3.52	119.49	123.31
1	1A	2604	PSU	O2-C2-N1	-3.51	119.17	122.79
1	1A	2445	2MG	C6-C5-N7	3.50	136.65	130.29
1	1A	2069	G7M	O6-C6-C5	-3.48	120.24	128.01
1	1A	2030	6MZ	N1-C2-N3	-3.46	123.35	128.58
1	1A	1618	6MZ	C4-C5-N7	-3.42	106.67	110.58
1	1A	746	PSU	O2-C2-N1	-3.37	119.31	122.79
1	1A	2503	2MA	C2-N1-C6	3.34	123.23	118.10
1	1A	1962	5MC	C5-C6-N1	-3.20	119.84	123.31
1	1A	2030	6MZ	C4-N9-C8	3.18	109.08	105.74
1	1A	2251	OMG	C6-C5-N7	3.16	136.05	130.29
1	1A	2552	OMU	O4-C4-C5	-3.13	119.76	125.16
1	1A	1618	6MZ	C6-C5-N7	3.13	135.84	132.43
1	1A	2503	2MA	C4-C5-N7	-3.08	107.06	110.58
1	1A	1835	2MG	C6-C5-N7	3.01	135.77	130.29
1	1A	2069	G7M	C3'-C2'-C1'	3.00	107.13	101.46
1	1A	2503	2MA	N6-C6-N1	2.98	121.05	117.03
1	1A	1618	6MZ	N1-C2-N3	-2.97	124.09	128.58
1	1A	2030	6MZ	C5-N7-C8	2.97	108.11	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1939	5MU	O2-C2-N1	-2.93	118.98	122.80
1	1A	747	5MU	O2-C2-N1	-2.91	119.01	122.80
1	1A	2445	2MG	N1-C2-N2	2.86	119.48	116.56
1	1A	2503	2MA	C4-N9-C8	2.69	108.56	105.74
1	1A	2030	6MZ	N9-C8-N7	-2.68	110.14	113.94
1	1A	2449	H2U	N3-C2-N1	2.65	119.31	116.65
1	1A	1962	5MC	C5-C4-N3	-2.65	119.04	121.75
1	1A	745	1MG	C4-C5-N7	-2.62	106.51	110.67
1	1A	2069	G7M	O4'-C1'-N9	2.59	114.23	108.36
1	1A	2445	2MG	C4-C5-N7	-2.58	106.59	110.67
1	1A	2605	PSU	C5-C6-N1	-2.55	118.60	122.14
1	1A	745	1MG	C6-C5-N7	2.53	134.97	129.36
1	1A	746	PSU	C5-C6-N1	-2.52	118.64	122.14
1	1A	2069	G7M	C5-C6-N1	2.50	117.01	111.84
1	1A	2580	PSU	C5-C6-N1	-2.50	118.67	122.14
1	1A	2251	OMG	C4-C5-N7	-2.49	106.72	110.67
1	1A	2069	G7M	O2'-C2'-C3'	-2.47	103.91	111.82
1	1A	2580	PSU	O4'-C1'-C2'	2.45	108.54	105.15
1	1A	1835	2MG	C4-C5-N7	-2.45	106.79	110.67
1	1A	2498	OMC	O2-C2-N3	-2.43	118.49	122.33
1	1A	1618	6MZ	C5-N7-C8	2.37	107.17	103.45
1	1A	1915	PSU	C5-C6-N1	-2.37	118.86	122.14
1	1A	955	PSU	C5-C6-N1	-2.36	118.86	122.14
1	1A	2449	H2U	O2-C2-N1	-2.36	120.27	123.10
1	1A	2503	2MA	C6-C5-N7	2.33	136.58	132.09
1	1A	2449	H2U	C5-C6-N1	-2.31	104.52	111.52
1	1A	2069	G7M	CN7-N7-C8	2.30	128.27	124.79
1	1A	1911	PSU	C5-C6-N1	-2.27	118.99	122.14
1	1A	2445	2MG	N2-C2-N3	-2.26	117.63	120.51
1	1A	1618	6MZ	C4-N9-C8	2.20	108.05	105.74
1	1A	2069	G7M	O3'-C3'-C2'	-2.18	104.82	111.82
1	1A	2445	2MG	O6-C6-C5	-2.16	120.84	126.53
1	1A	2457	PSU	C5-C6-N1	-2.15	119.15	122.14
1	1A	2503	2MA	C5-N7-C8	2.14	106.81	103.45
1	1A	2552	OMU	O2-C2-N1	-2.13	120.02	122.80
1	1A	1917	PSU	C5-C6-N1	-2.13	119.19	122.14
1	1A	2604	PSU	C5-C6-N1	-2.12	119.19	122.14
1	1A	2251	OMG	O6-C6-C5	-2.09	121.00	126.53
1	1A	2069	G7M	C2-N1-C6	-2.09	121.31	125.11
1	1A	2504	PSU	C6-C5-C4	-2.09	116.76	118.17
1	1A	1835	2MG	O6-C6-C5	-2.07	121.07	126.53
1	1A	2445	2MG	CM2-N2-C2	-2.03	119.28	123.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2457	PSU	O4'-C1'-C2'	2.01	107.93	105.15

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	746	PSU	C2'-C1'-C5-C4
1	1A	746	PSU	C2'-C1'-C5-C6
1	1A	746	PSU	O4'-C1'-C5-C6
4	1E	150[B]	MEQ	C-CA-CB-CG
4	1E	150[B]	MEQ	CG-CD-NE2-CE
4	1E	150[B]	MEQ	OE1-CD-NE2-CE
4	1E	150[A]	MEQ	NE2-CD-CG-CB
4	1E	150[A]	MEQ	OE1-CD-CG-CB
4	1E	150[B]	MEQ	CA-CB-CG-CD
1	1A	2030	6MZ	O4'-C4'-C5'-O5'
1	1A	2030	6MZ	C3'-C4'-C5'-O5'
1	1A	747	5MU	C3'-C4'-C5'-O5'
1	1A	746	PSU	O4'-C1'-C5-C4
1	1A	2445	2MG	C3'-C4'-C5'-O5'
1	1A	2503	2MA	O4'-C4'-C5'-O5'
1	1A	2504	PSU	O4'-C4'-C5'-O5'
1	1A	2503	2MA	C4'-C5'-O5'-P
1	1A	1835	2MG	C3'-C4'-C5'-O5'
1	1A	2069	G7M	O4'-C4'-C5'-O5'
1	1A	1962	5MC	O4'-C1'-N1-C6
1	1A	1835	2MG	O4'-C4'-C5'-O5'
1	1A	1962	5MC	C2'-C1'-N1-C6

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	2251	OMG	1	0
1	1A	747	5MU	2	0
1	1A	2604	PSU	1	0
1	1A	2069	G7M	3	0
1	1A	1939	5MU	1	0
1	1A	2498	OMC	1	0
1	1A	2030	6MZ	1	0
4	1E	150[A]	MEQ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
56	6UQ	1A	3001	1	101,105,105	1.61	14 (13%)	130,164,164	2.02	39 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	6UQ	1A	3001	1	-	15/47/211/211	0/11/11/11

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	1A	3001	6UQ	OCP-CCJ	6.29	1.47	1.40
56	1A	3001	6UQ	CDF-CAC	-5.53	1.40	1.51
56	1A	3001	6UQ	OBQ-CBP	5.12	1.55	1.43
56	1A	3001	6UQ	CAD-CAJ	-4.28	1.40	1.50
56	1A	3001	6UQ	OCS-CCR	3.74	1.47	1.41
56	1A	3001	6UQ	CCM-CCL	-3.38	1.48	1.54
56	1A	3001	6UQ	OCP-CCO	3.28	1.48	1.44
56	1A	3001	6UQ	OCQ-CCR	3.25	1.46	1.41
56	1A	3001	6UQ	OBE-CAX	3.06	1.46	1.41
56	1A	3001	6UQ	OCG-CCB	3.04	1.48	1.41
56	1A	3001	6UQ	OAL-CAM	2.21	1.48	1.44
56	1A	3001	6UQ	O1-C1	2.11	1.47	1.41
56	1A	3001	6UQ	OAY-CAX	2.09	1.43	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	1A	3001	6UQ	CBC-CBD	-2.09	1.49	1.53

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1A	3001	6UQ	CCC-OCH-CCU	-7.60	105.14	117.76
56	1A	3001	6UQ	CBC-CBF-CBG	-6.43	104.14	114.99
56	1A	3001	6UQ	OCI-CCD-CCE	-4.64	97.02	103.48
56	1A	3001	6UQ	CCZ-CCO-CCN	-4.30	104.75	115.31
56	1A	3001	6UQ	O1-CCB-OCG	4.18	117.57	108.92
56	1A	3001	6UQ	OCK-CCE-CCD	-4.03	97.00	103.54
56	1A	3001	6UQ	CDG-CAR-CAM	-4.00	107.44	113.39
56	1A	3001	6UQ	OBBCBC-CDJ	3.95	115.78	108.61
56	1A	3001	6UQ	CAP-OAS-CAU	-3.74	107.27	114.72
56	1A	3001	6UQ	O1-C1-C2	3.57	116.02	109.09
56	1A	3001	6UQ	CAF-CAA-CAB	3.53	121.57	117.78
56	1A	3001	6UQ	OBBCBC-CBD	-3.37	97.39	102.03
56	1A	3001	6UQ	CAP-OAQ-CAR	-3.33	104.69	113.82
56	1A	3001	6UQ	CAA-CAF-CLAG	3.31	122.11	118.09
56	1A	3001	6UQ	CAX-OAY-CAZ	-3.20	109.25	112.16
56	1A	3001	6UQ	CCF-CCE-CCD	-3.01	106.90	112.56
56	1A	3001	6UQ	OAY-CAZ-CDH	2.99	109.58	105.94
56	1A	3001	6UQ	OBBCBC-CBF	2.97	115.57	109.38
56	1A	3001	6UQ	CDF-CAC-CAB	-2.92	115.94	121.23
56	1A	3001	6UQ	CDJ-CBC-CBF	-2.92	107.17	111.85
56	1A	3001	6UQ	OBE-CBD-CBI	2.78	113.68	108.20
56	1A	3001	6UQ	CDK-CBM-CBL	-2.75	109.29	113.39
56	1A	3001	6UQ	O2-C2-C3	-2.75	104.10	110.39
56	1A	3001	6UQ	CDM-ODL-CBL	-2.71	107.51	114.47
56	1A	3001	6UQ	CDE-ODD-CAE	-2.67	107.49	114.74
56	1A	3001	6UQ	CAA-CAB-CAC	-2.64	119.84	122.65
56	1A	3001	6UQ	O4-CBO-OBN	-2.60	103.84	110.69
56	1A	3001	6UQ	CDH-CAZ-CAU	-2.58	109.55	113.39
56	1A	3001	6UQ	OCQ-CCL-CCM	-2.55	98.58	105.36
56	1A	3001	6UQ	OCP-CCO-CCN	2.51	113.16	109.79
56	1A	3001	6UQ	OCH-CCU-CCV	2.46	115.68	111.14
56	1A	3001	6UQ	CAA-CAB-CLAI	2.46	121.07	118.09
56	1A	3001	6UQ	C3-C4-C5	-2.38	105.65	110.93
56	1A	3001	6UQ	CBK-CBL-CBM	-2.33	107.07	110.31
56	1A	3001	6UQ	O4-C4-C3	2.30	113.07	107.23
56	1A	3001	6UQ	C1-O1-CCB	-2.14	110.49	114.33
56	1A	3001	6UQ	OCS-CCM-CCL	-2.10	99.76	105.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1A	3001	6UQ	O4-C4-C5	2.09	114.97	109.48
56	1A	3001	6UQ	OAQ-CAR-CAM	2.01	112.91	109.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

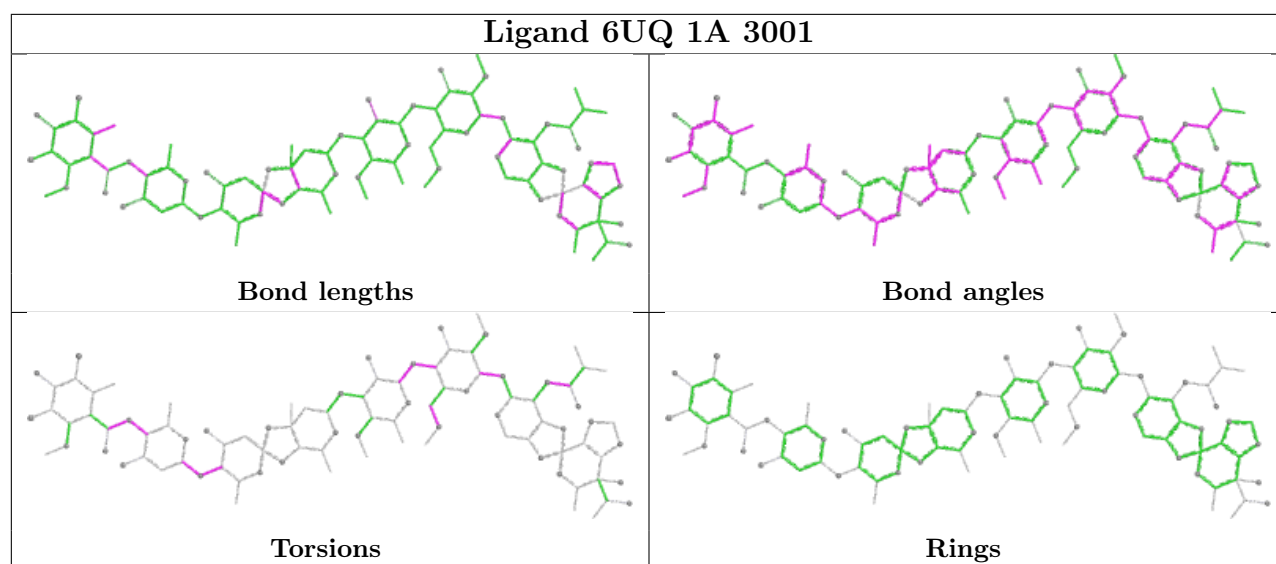
Mol	Chain	Res	Type	Atoms
56	1A	3001	6UQ	C2-C1-O1-CCB
56	1A	3001	6UQ	C3-C4-O4-CBO
56	1A	3001	6UQ	CAD-CAJ-OAL-CAM
56	1A	3001	6UQ	CCV-CCU-OCH-CCC
56	1A	3001	6UQ	OCY-CCU-OCH-CCC
56	1A	3001	6UQ	OAK-CAJ-OAL-CAM
56	1A	3001	6UQ	OAQ-CAP-OAS-CAU
56	1A	3001	6UQ	CAO-CAP-OAS-CAU
56	1A	3001	6UQ	CAR-CAM-OAL-CAJ
56	1A	3001	6UQ	CAN-CAM-OAL-CAJ
56	1A	3001	6UQ	C5-C6-O6-CDO
56	1A	3001	6UQ	CAZ-CAU-OAS-CAP
56	1A	3001	6UQ	OBN-CBO-O4-C4
56	1A	3001	6UQ	CBP-CBO-O4-C4
56	1A	3001	6UQ	CAV-CAU-OAS-CAP

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	1A	3001	6UQ	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

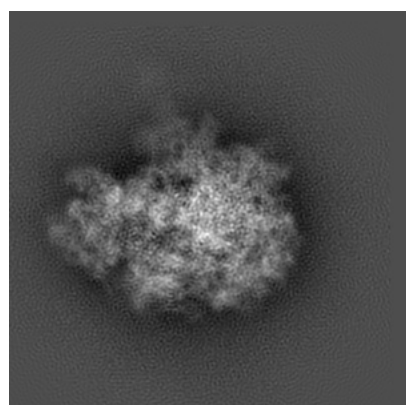
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8237. These allow visual inspection of the internal detail of the map and identification of artifacts.

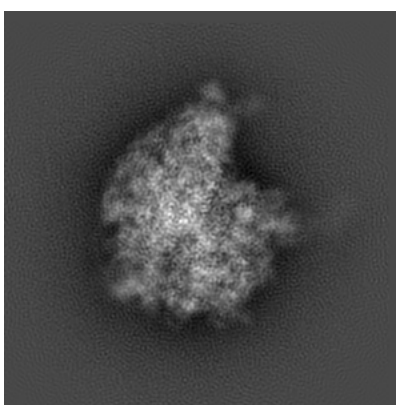
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

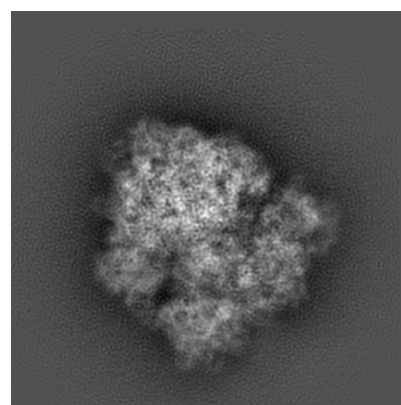
6.1.1 Primary map



X



Y

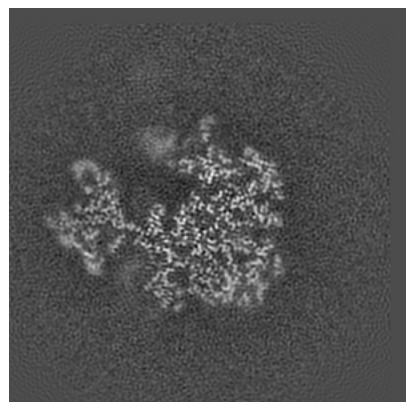


Z

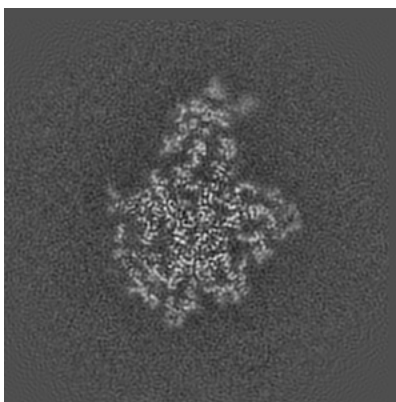
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

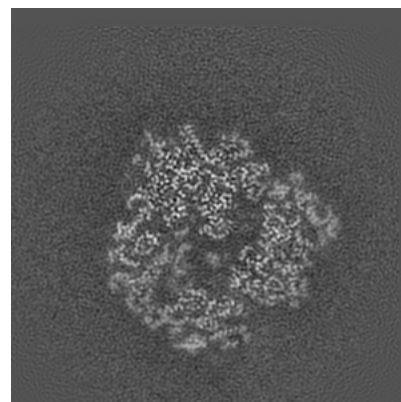
6.2.1 Primary map



X Index: 184



Y Index: 184

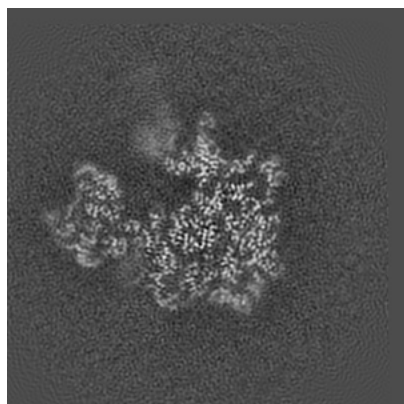


Z Index: 184

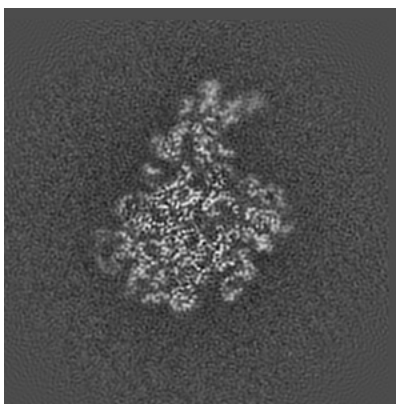
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

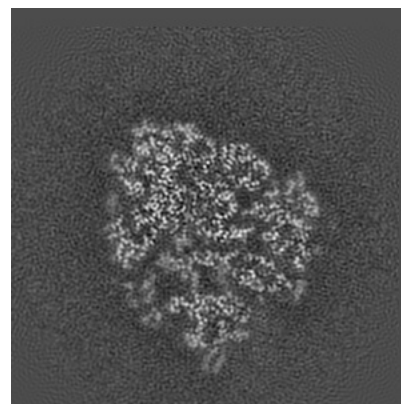
6.3.1 Primary map



X Index: 179



Y Index: 175

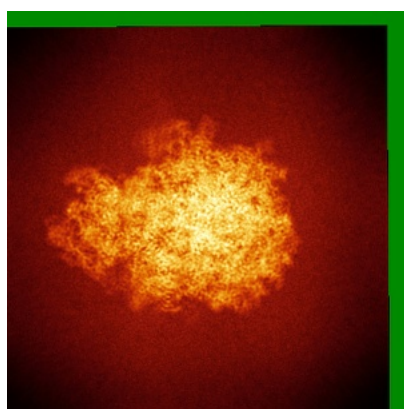


Z Index: 177

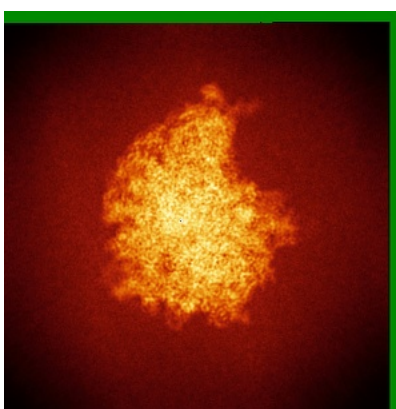
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

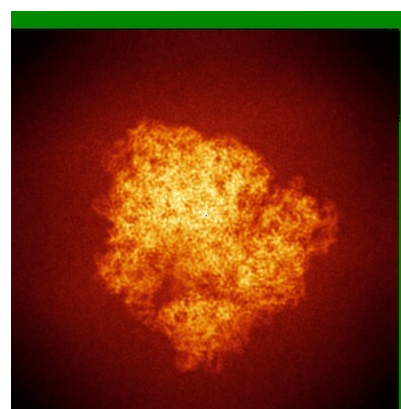
6.4.1 Primary map



X



Y

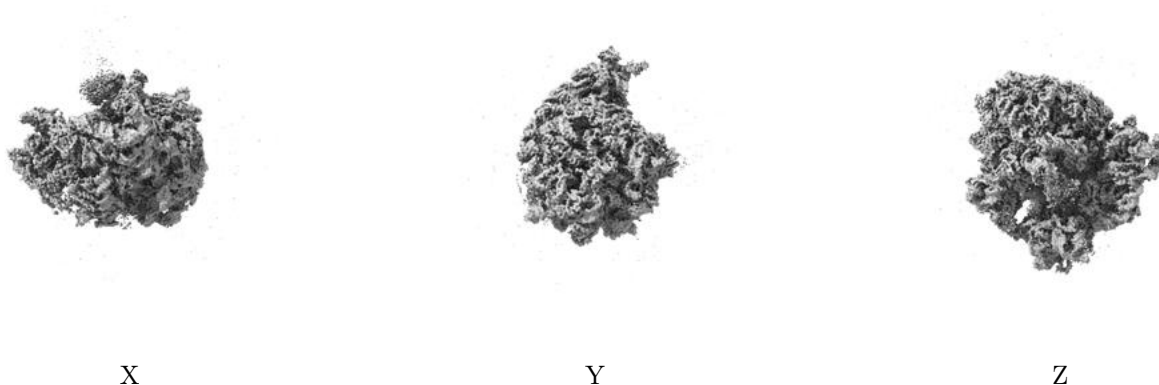


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.000801. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

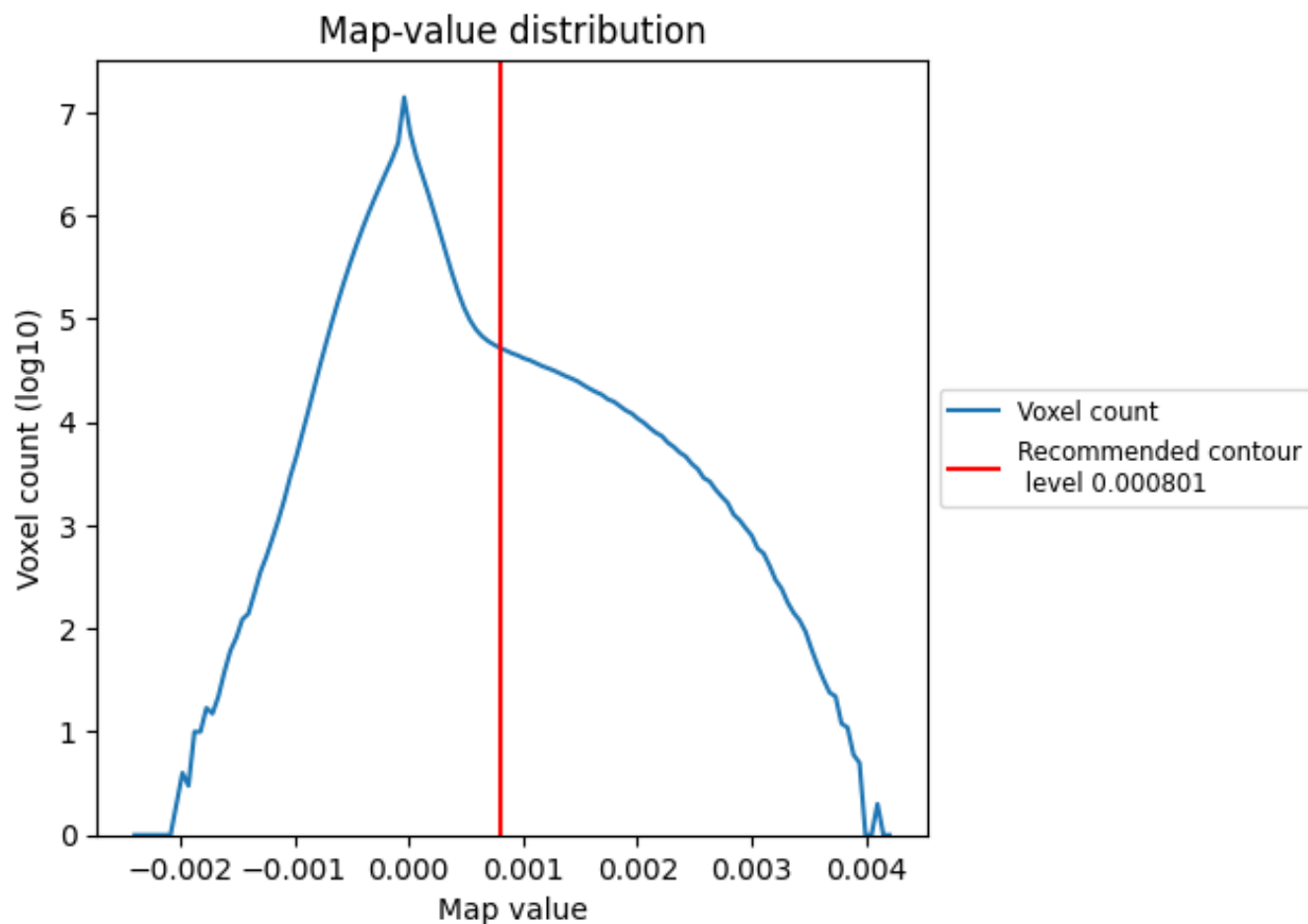
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

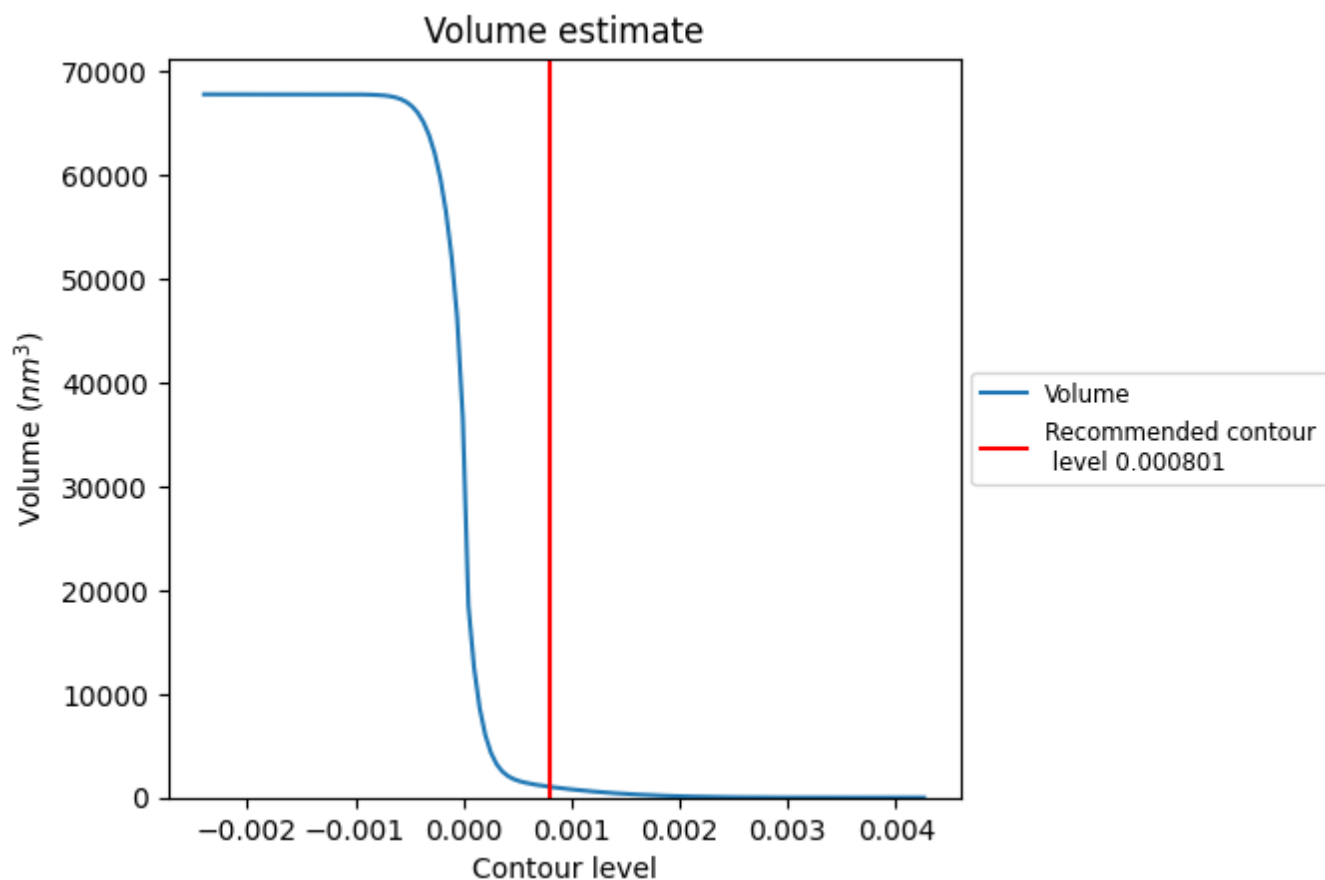
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

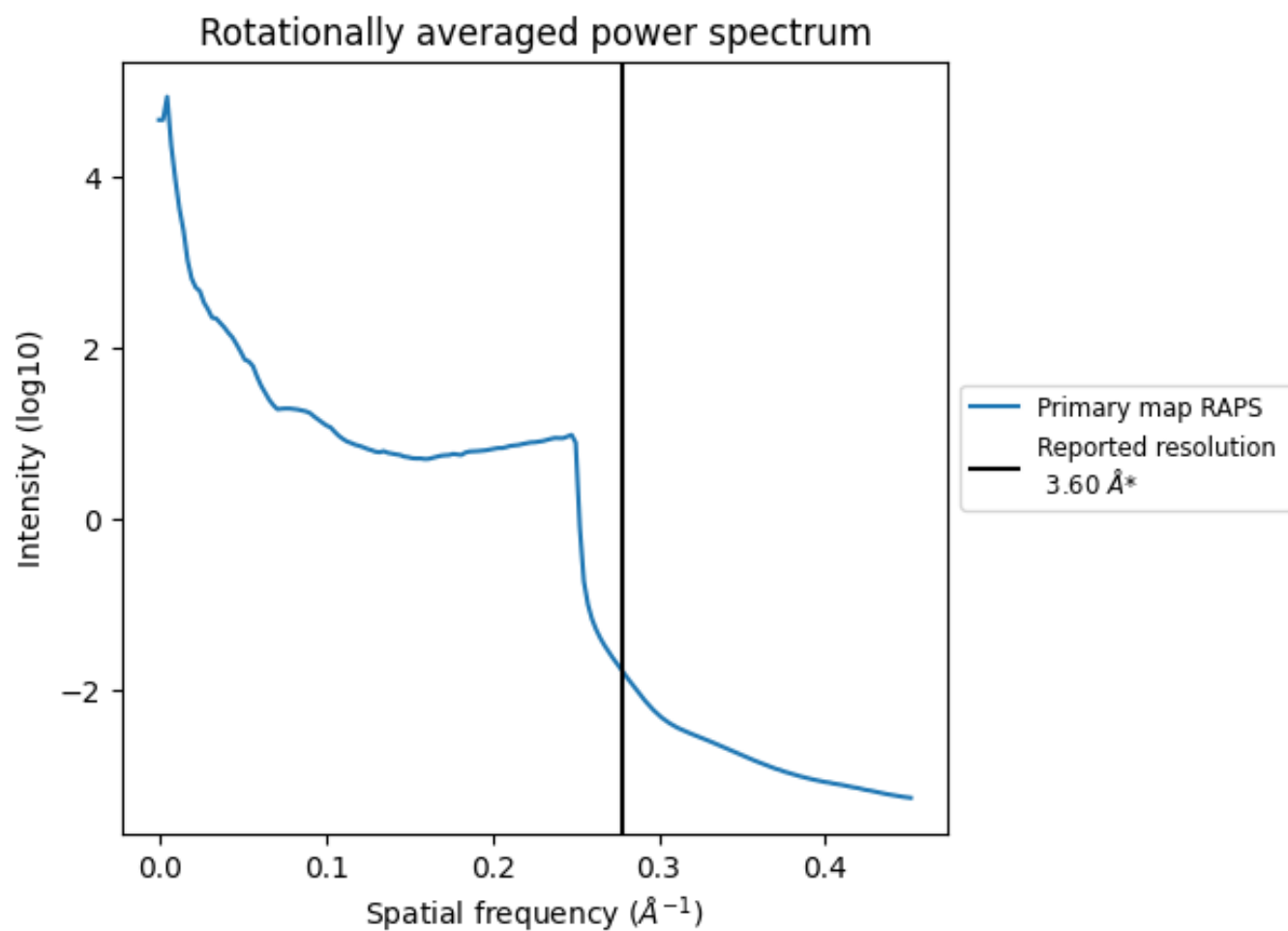
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1035 nm³; this corresponds to an approximate mass of 935 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

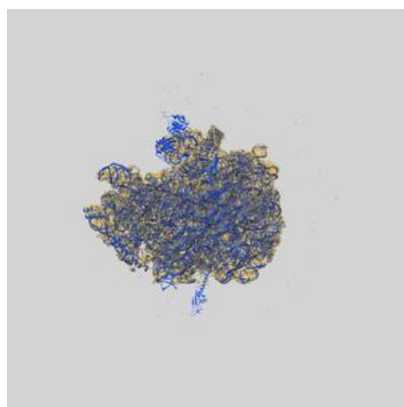
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

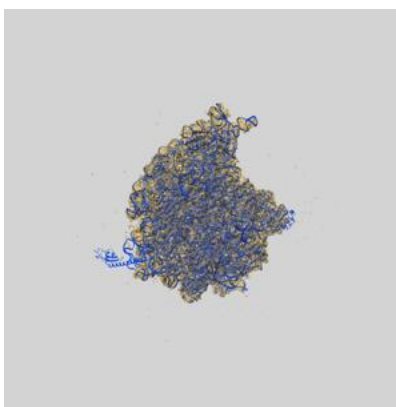
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8237 and PDB model 5KCR. Per-residue inclusion information can be found in section [3](#) on page [15](#).

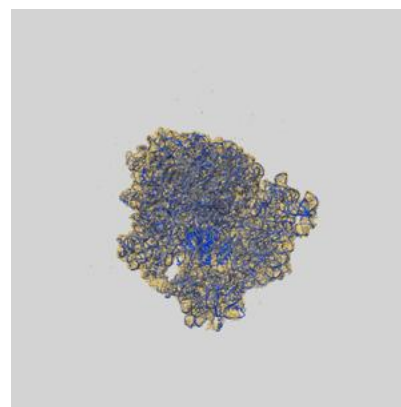
9.1 Map-model overlay [i](#)



X



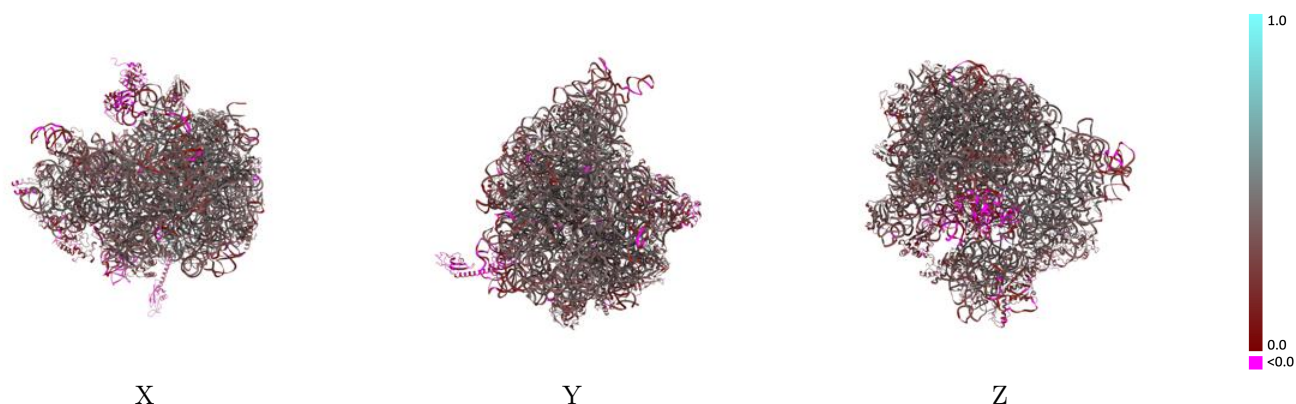
Y



Z

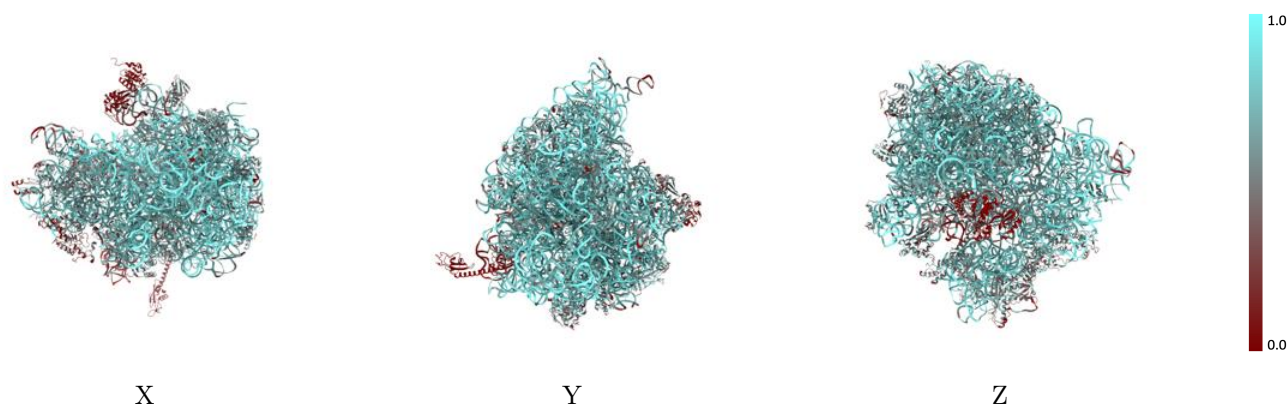
The images above show the 3D surface view of the map at the recommended contour level 0.000801 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



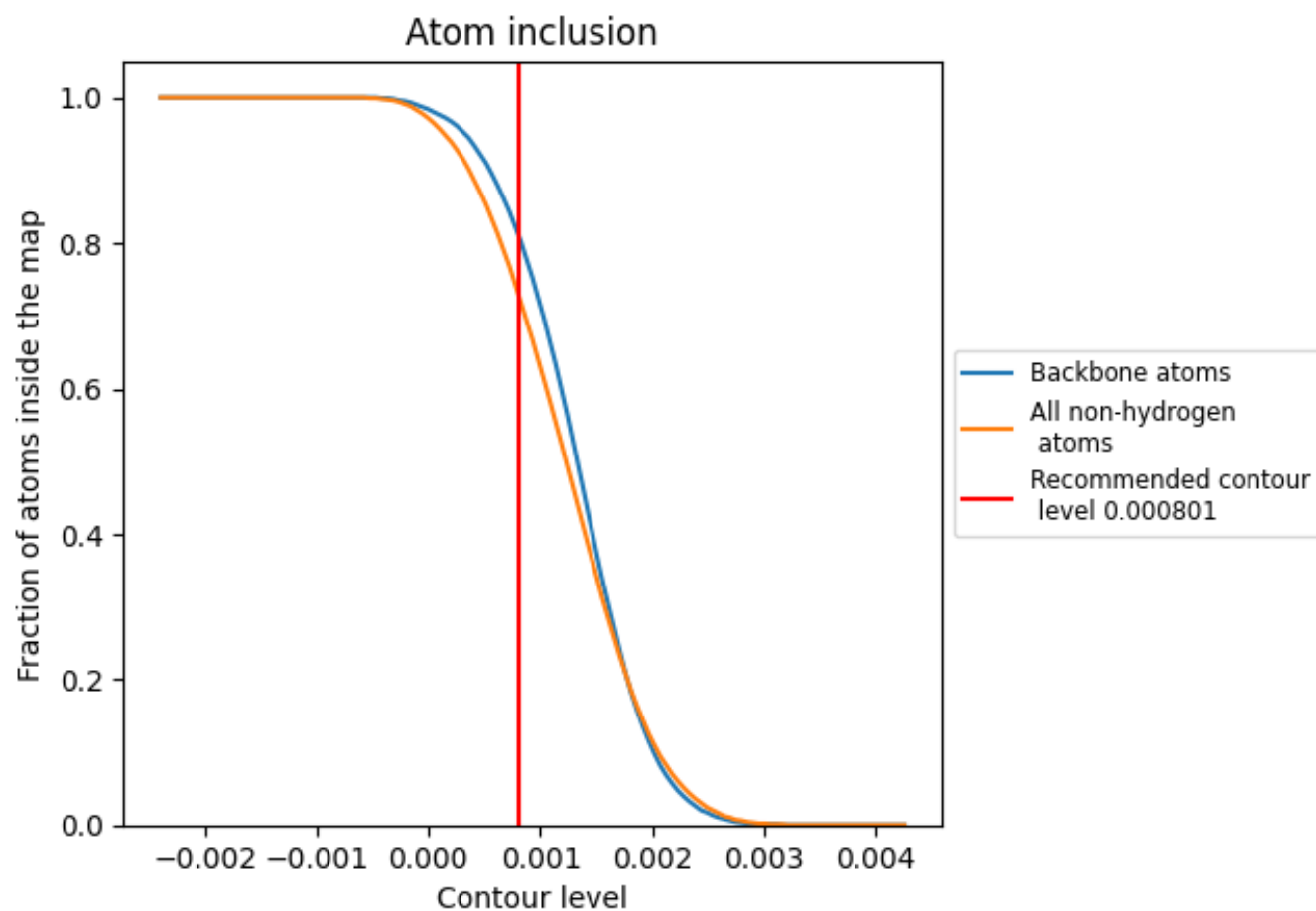
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.000801).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.000801) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7310	 0.3460
10	 0.6440	 0.3860
11	 0.6220	 0.3870
12	 0.5810	 0.3060
13	 0.6480	 0.3530
15	 0.6380	 0.3700
16	 0.0890	 0.2680
17	 0.6620	 0.3850
18	 0.6600	 0.4210
19	 0.6350	 0.3780
1A	 0.8190	 0.3620
1B	 0.8400	 0.3410
1D	 0.6640	 0.4220
1E	 0.6320	 0.3860
1F	 0.5760	 0.3480
1G	 0.4850	 0.1980
1H	 0.5200	 0.2800
1I	 0.0570	 0.0530
1J	 0.0210	 0.0330
1K	 0.0650	 0.0660
1N	 0.6450	 0.3820
1O	 0.5890	 0.3850
1P	 0.6190	 0.3820
1Q	 0.6450	 0.4050
1R	 0.6510	 0.3740
1S	 0.6290	 0.3100
1T	 0.6060	 0.3660
1U	 0.6960	 0.3960
1V	 0.6300	 0.3580
1W	 0.6080	 0.3870
1X	 0.5480	 0.3320
1Y	 0.5820	 0.3280
1Z	 0.6130	 0.3150
1a	 0.8330	 0.3660
1b	 0.2620	 0.1940



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Chain	Atom inclusion	Q-score
1c	 0.5330	 0.3340
1d	 0.5430	 0.3100
1e	 0.6000	 0.3560
1f	 0.5350	 0.2650
1g	 0.4540	 0.2570
1h	 0.5980	 0.3520
1i	 0.5560	 0.2820
1j	 0.4320	 0.2610
1k	 0.5470	 0.3110
1l	 0.6180	 0.3710
1m	 0.5550	 0.3080
1n	 0.6180	 0.3260
1o	 0.6140	 0.3360
1p	 0.6110	 0.3480
1q	 0.5630	 0.3220
1r	 0.6190	 0.3260
1s	 0.5570	 0.3070
1t	 0.6230	 0.3160
1u	 0.1650	 0.1750
1v	 0.9330	 0.4890
1x	 0.5880	 0.2480